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# A Relative Risk Ranking of Selected Substances on the National Pollutant Release Inventory

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**Atlantic Region**



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# A Relative Risk Ranking of Selected Substances on the National Pollutant Release Inventory

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## ABSTRACT

The National Pollutant Release Inventory (NPRI) provides pollutant release and transfer data from point sources to various media in the Canadian environment. While the inventory serves as Canada's community right-to-know program, the growing number of listed substances and reporting facilities makes it exceedingly difficult for the public to discern which substances are of greatest concern in their respective communities. A chemical's impact is best characterized when its environmental release data is combined with its toxicity and environmental fate properties. Presently, the NPRI does not provide a synthesis of this critical information and there is a need to provide more context with NPRI data to increase its usability. To help deliver this context and guide future internal priority setting, a relative risk ranking has been compiled for a subset of NPRI substances using a modified Chemical Hazard and Evaluation Management Strategies (CHEMS) model. By making use of the paradigm, Risk = Toxicity x Exposure, the model combines toxicity, chemical fate properties and NPRI release data to yield a risk score for each substance. The resulting risk scores are ranked accordingly to provide a priority ranking of the substances. While the model makes use of toxicity and exposure data, the risk ranking produced does not represent a risk assessment. Limitations included the reliance on modelled data and default values to fill data gaps and uncertain reliability in reported NPRI data. In spite of its limitations, it is believed the CHEMS risk ranking scheme provides a useful tool for prioritizing NPRI substances.

## RÉSUMÉ

L'Inventaire national des rejets de polluants (INRP) fournit des données sur les rejets et les transferts de polluants de sources ponctuelles dans l'environnement au Canada. L'inventaire sert au programme du droit de savoir de la collectivité Canadien. Cependant, en raison du nombre croissant de substances répertoriées et d'installations tenues de produire des déclarations, il est très difficile pour les Canadiens de déterminer quelles substances sont les plus préoccupantes dans leur collectivité. On peut mieux déterminer l'impact d'une substance chimique en combinant les données sur le rejet de la substance dans l'environnement, sa toxicité et son évolution dans l'environnement. Actuellement, l'INRP ne met pas en rapport ces renseignements essentiels. On doit fournir davantage de contexte avec les données de l'INRP pour en accroître la convivialité. Afin de fournir ce contexte et d'orienter l'établissement des priorités futures à l'interne, on a effectué, à l'aide d'une version modifiée du modèle CHEMS (*Chemical Hazard and Evaluation Management Strategies*), un classement des risques relatifs pour un sous-ensemble de substances de l'INRP. En utilisant le paradigme *Risque = Toxicité x Exposition*, le modèle allie de l'information sur la toxicité et l'évolution dans l'environnement aux données sur les rejets contenues dans l'INRP pour établir une cote de risque pour chaque substance. Ces cotes de risque permettent de classer les substances par ordre de priorité. Bien que le modèle utilise des données sur la toxicité et l'exposition, la cote de risque obtenue ne constitue pas une évaluation du risque. Le modèle comporte des limites, notamment la fiabilité des données modélisées et des valeurs de remplacement servant à combler les lacunes en matière de données et la variabilité des données déclarées aux fins de l'INRP. Malgré ces limites, le système d'établissement de cotes de risque à l'aide du modèle CHEMS est un outil utile pour classer les substances de l'INRP par ordre de priorité.

## ACKNOWLEDGEMENTS

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## 1.0 INTRODUCTION

The National Pollutant Release Inventory (NPRI) was established in 1993 by Environment Canada in response to public demands to have access to industrial pollutant information. The purpose of the NPRI is to provide Canadians with comprehensive, national data on quantities of pollutants released, disposed and transferred by facilities operating in Canada. Under the authority of CEPA 1999, facilities that meet specific reporting criteria are required to submit an annual report to Environment Canada summarizing their pollutant releases and transfers. Currently, the inventory is comprised of 303 substances of concern and recent statistics indicate more than 8400 facilities report to the program.

The inventory of data, publicly accessible through Environment Canada's web site <http://www.ec.gc.ca/pdb/npri >, provides Canadians with pollutant releases to the environment on a per facility basis. Environment Canada also issues an annual National Overview report which provides a summary of pollutant releases and transfers to the Canadian environment, including pollutant release trends and profiles of substances released and transferred in the largest quantities through "top ten" lists. While these reports provide invaluable information on pollution sources in Canada and quantities of pollutants released to the Canadian environment, they nonetheless fall short of the public's desire for meaningful interpretation of the data.

A chemical's impact is better understood when its environmental releases are combined with its toxicity and environmental fate properties. Presently, the overview reports published by Environment Canada do not provide a synthesis of this critical information and there is, therefore, a need to place NPRI data within the context of environmental and health risks to increase its utility. To this end, Environment Canada, Atlantic Region has initiated efforts and provided greater context for NPRI data through the application of the Chemical Hazard and Evaluation for Management Strategies (CHEMS) model. The CHEMS model is an example of an algorithm which combines environmental releases, toxicity, and chemical fate properties to yield a priority ranking for a group of chemicals based on risk (Swanson *et al.* 1997). The model was originally developed by researchers at the University of Tennessee to compile a risk ranking for the U.S. Toxic Release Inventory and was used by Environment Canada, Atlantic Region to develop a priority ranking of NPRI substances released to the Atlantic environment (Environment Canada 2000). By providing a ranking of NPRI substances according to the relative risk they pose, the CHEMS model can guide internal priority setting of government programs aimed at reducing overall environmental risk and help Canadians understand the environmental risk of specific chemicals.

As an expansion of the Environment Canada work described above, Atlantic Region recently compiled a relative risk ranking for NPRI by applying a modified version of the CHEMS model. In contrast to the previous Environment Canada report, this evaluation goes beyond an Atlantic Region focus by providing national, provincial and territorial relative risk rankings for each province and territory. In addition, through modifications to the CHEMS model and by incorporating advances made in the science of categorizing substances for priority setting, this work attempts to overcome some of the limitations identified by the scientific and regulated community regarding Atlantic Region's use of CHEMS in its initial priority ranking of the NPRI. The following report details the risk ranking compiled for NPRI using 2003 data, including an overview of the CHEMS model, a description of the data collection procedure, data treatment, the risk ranking results and the model's limitations and uncertainties.

## 2.0 MODEL OVERVIEW

The CHEMS model combines toxicity and exposure endpoints to yield a relative risk ranking for a group of substances. Following the general paradigm of "risk = toxicity x exposure", a risk score is calculated by multiplying the sum of release-weighted toxicity endpoints by the sum of exposure endpoints:

*Risk Score* = [sum of release-weighted toxicity endpoints] x [sum of exposure endpoints]

When risk scores have been calculated for all substances in a group, the substances can be ranked accordingly; the higher ranked substances will pose a higher risk, while lower ranked substances will present a lower risk to the environment. Although the model makes use of measured and estimated toxicity and environmental fate values, the CHEMS risk ranking scheme does not represent a detailed risk assessment and should not be construed as such. Rather, the resultant quantitative risk ranking can be best used to identify priority substances for further study and evaluation and such scoring systems are generally regarded as the first tier of risk assessment (Solomon 1999).

### 2.1 Toxicity and Fate Measures

The modified CHEMS model employed by Environment Canada used six toxicity and three fate parameters to determine the overall risk of a substance (Table 1). Bioaccumulation, persistence and NPRI environmental release amounts are the three fate parameters included to represent a substance's exposure potential.

**Table 1**: Parameters used by modified CHEMS model to represent exposure potential, human health and environmental effects

| Effect / Parameter | Endpoint | Definition |
|---|---|---|
| HUMAN HEALTH | | |
| Acute Oral | Rat Oral $LD_{50}$ | The quantity of a substance, expressed as the mass of substance per mass of test animal (mg/kg), which causes 50% mortality in a group of test animals within 14 days given a single oral dose. |
| Acute Inhalation | Rat Inhalation $LC_{50}$ | The concentration of a substance in air, expressed in mg/L, which causes 50% mortality in a group of test animals when inhaled continuously for 4 hours. |
| Chronic | Carcinogenicity | Based on United States Environmental Protection Agency (US EPA) and International Agency for Research on Cancer (IARC) classifications. |
| Chronic | Non-cancer | Based on the Reference Dose (RfD) or Reference Concentration (RfC). The RfD or RfC is the lifetime, average daily dose or concentration of a substance an individual can be exposed to without suffering adverse affects. RfDs and RfCs are normally determined by dividing the no-observable adverse effect level or concentration (NOAEL/NOAEC) in a chronic animal study by an uncertainty factor of 100 to account for intraspecies and interspecies variation. The NOAEL/NOAEC represents the highest test concentration that does not show any deleterious effects in the test animals exposed daily for up to 2 years. |
| ENVIRONMENTAL | | |
| Acute aquatic | Fish 96-hour $LC_{50}$ | The concentration of a substance in water (mg/L) which causes 50% mortality in a group of test fish (*Pimephales promelas* - fathead minnow) exposed continuously for 96 hours. |
| Acute aquatic | Water Flea 48-hour $LC/EC_{50}$ | The concentration of a substance in water (mg/L) which causes 50% mortality or immobilization in a group of test animals (*Daphnia magna*) exposed continuously for 48 hours. |
| EXPOSURE POTENTIAL | | |
| Persistence | Reaction Half-life | Reaction half-life is the time required for a substance to degrade to half its original concentration taking into consideration how it partitions in the environment, its respective half-lives in each environmental media (e.g. air, water, soil, sediment) and intermedia transport. This parameter was estimated by Level III fugacity modelling available through EPI Suite v3.12.[a] |
| Bioaccumulation/ Bioconcentration | Aquatic Bioaccumulation Factor (BAF) or Bioconcentration Factor (BCF) | Bioaccumulation factor (BAF) is the ratio of the concentration of a substance in an aquatic organism to the concentration in water, based on uptake from the surrounding medium and food. Bioconcentration factor (BCF) is the ratio of the concentration of a substance in an organism to the concentration in water, based only on uptake from the surrounding medium. When measured BAF/BCF data were not available, BCF was estimated using a quantitative structure-activity relationship (QSAR). |
| Release Amount | Release Weighting Factors (RWFs) | Calculated for each substance for each medium using the quantity of substance released to air, water and land reported to the 2003 NPRI. |

[a] EPI Suite v3.12 is a collection of quantitative structure-activity relationship (QSAR)-based software that provides estimates for a number of environmental fate properties.

## 2.2 Substance Selection

The first risk ranking conducted by Atlantic Region included all substances listed on the NPRI. However, since some of the model parameters are not particularly relevant to metals (e.g. reaction half-life, bioaccumulation), the metals were removed from this risk ranking exercise. This approach was supported by Environment Canada's protocol for categorizing metals on the domestic substance list (DSL).[1]

The toxicological and fate data used in the previous risk ranking effort was never subjected to a critical review and was derived from many unverified references and old data. As such, the toxicological and fate database was completely reviewed to build a robust data set for the current risk ranking. In the interest of making the data collection step less onerous, the NPRI list was reduced by applying some screening criteria. Substances that were either reported by 5 or more facilities *or* whose cumulative releases to the environment were greater than 10 tonnes in 2003 were included in the current risk ranking report. Based on these criteria, the final data set included 99 organic and non-metallic inorganic substances. Again, non-metallic inorganic substances were included in the subset and not metals since separate guidance has been developed for metal containing substances and the DSL guidance manual recommends grouping non-metallic inorganics with the organics for the purpose of DSL categorization.

# 3.0 DATA SOURCES AND TREATMENT

A considerable effort was made to compile a comprehensive database of measured toxicity and chemical fate data from reputable sources for all NPRI substances included in the ranking. Data gathering was assisted by Environment Canada's Existing Substances Branch (ESB) who shared data they had collected for the purpose of DSL categorization. A number of reliable sources were consulted for chemical toxicity and fate information as described below.

## 3.1 Effects Data

The majority of health and ecotoxicity data were obtained from monographs provided by the US EPA's Integrated Risk Information System (IRIS), International Agency for Research on Cancer (IARC), Agency for Toxic Substances and Disease Registry (ATSDR), Hazardous Substances Data Bank (HSDB), European Chemical Bureau's International Uniform ChemicaL Information Database (IUCLID), Canada's Centre for Occupational Health and Safety CHEMpendium Collection (CESARS, CHEMINFO), International Programme on Chemical Safety (Environmental Health Criteria), Priority Substance List (PSL) assessment reports and the US EPA's ECOTOX database. When measured data were unavailable, quantitative structure-activity relationships (QSARs), Expert judgement or default values were used to assign a value to each toxicity parameter.

[1] The Existing Substances Branch (ESB) of Environment Canada is tasked with categorizing the 23,000 substances on the DSL by 2006. Organic and non-metal-containing inorganic substances will be categorized on the basis of persistence, bioaccumulation and inherent toxicity whereas metals will be primarily categorized on the basis of inherent toxicity.

### *3.1.1 Acute rat oral and inhalation toxicity*

Acute rat oral $LD_{50}$ values and inhalation $LC_{50}$ values were primarily obtained from HSDB, CHEMINFO, CESARS, and IUCLID. When more than one toxicity value was obtained for a chemical, the geometric mean was taken of all the values. The geometric mean, rather than the arithmetic mean, was used for all toxicity endpoints since the distribution of sensitivities of individual organisms in toxicity tests on most materials are more likely to be log normal than normal (US EPA 1995). In instances where the exposure period for the rat inhalation study was not equivalent to four hours, the $LC_{50}$ values were scaled to 4-hour exposures according to the following formula recommended by CHEMS (Swanson *et al.* 1997):

$$\textit{4-hr } LC_{50} = \text{t-hr } LC_{50} \times t/4$$

In a few cases, when no acute rat inhalation toxicity information was available, chronic data (*i.e.* time-weighted average exposure limit[2]) or inhalation data from another species (mouse) was used to represent the $LC_{50}$ for the chemical.

When no inhalation data were available from any sources, the following equation was used to estimate inhalation toxicity from oral toxicity (Green Seal 2005):

$$LC_{50} = \frac{\text{oral } LD_{50} \times ABS_{GI} \times BW}{ABS_{inh} \times R \times ET \times CF}$$

Where,
Oral $LD_{50}$ = single dose $LD_{50}$ for oral pathway
$ABS_{GI}$ = gastrointestinal absorption rate (0.8)
BW = animal body weight (0.35 kg)
$ABS_{inh}$ = inhalation absorption rate, unitless (1.0)
R = respiration rate for experimental animal (0.14 L/min)
ET = exposure time (4 h)
CF = conversion factor (60 min/h)

Lastly, in some cases when oral or inhalation toxicity information was lacking, these endpoints were assigned a value of zero if ingestion or inhalation could be ruled out as an exposure pathway. This was determined by reviewing the physical-chemical properties of the chemical (e.g. vapour pressure, Henry's Law constant), its NPRI distribution (*i.e.* percentages released to air, land and water) and environmental partitioning predicted by Level III fugacity modelling[3]. For example, if a chemical was determined to be a gas at room temperature, its Henry's Law constant predicted rapid volatilization and its NPRI distribution was 100% to air, then oral ingestion was ruled out as an exposure pathway. Similarly, if a chemical was shown to be a solid at room temperature, had very low volatilization potential and its NPRI distribution was mostly to land and water, then inhalation was ruled out as an exposure pathway and a zero was assigned for inhalation toxicity.

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[2] The time-weighted exposure limit is the time-weighted average concentration of a chemical in air for a normal 8-hour work day and 40-hour work week to which nearly all workers may be exposed day after day without harmful effects.

[3] Level III Fugacity modelling is a mass-balance approach that predicts a chemical's partitioning between 4 media (soil, sediment, air, water), according to its physical-chemical properties, reaction half-lives, intermedia transport velocities and advection rates under non-equilibrium conditions. See Appendix 1 for more information on fugacity modelling.

### 3.1.2 Carcinogenicity rating

Carcinogenicity ratings were obtained from IARC or IRIS. When a carcinogenicity rating was not available from either of the cited sources, the carcinogenicity rating for surrogate chemicals or supporting information from PSL Assessments and HSDB were used to assign a rating following the principles outlined by IARC and EPA. When no information was available, a default value was assigned to the chemical for its carcinogenicity rating.

### 3.1.3 Chronic non-cancer effect

The latest version of CHEMS includes the oral and inhalation No Observed Adverse Effect Level (NOAEL) as the chronic non-cancer effect (Swanson 2000a). The NOAEL is usually divided by a safety factor of 100 to yield a Reference Dose (RfD) or Reference Concentration (RfC) which is the average, lifetime daily dose a human can be exposed to without experiencing any deleterious effects. Occasionally, when uncertainties are present in the toxicological database (e.g. database incomplete, NOAEL not established, subchronic test used to establish NOAEL, increased sensitivity in the young), the NOAEL is divided by a safety factor greater than 100 to yield the RfD or RfC. In addition, some NOAELs are based on human occupational studies or scaled to human equivalent concentrations. As such, NOAELs are not always comparable across substances. Therefore, to allow for more consistent comparison between substances, the RfD and RfC was used in place of the oral and inhalation NOAEL to represent the chronic non-cancer effect.

Reference doses and concentrations were readily available from IRIS and ATSDR. When reference values were not available from these sources, supporting information from HSDB, PSL assessments, National Toxicology Program (NTP) reports and CHEMINFO was used to set an appropriate RfD or RfC. When both reference values were available, the more relevant exposure pathway was chosen based on NPRI distribution and environmental partitioning as determined by Level III fugacity modelling.

### 3.1.4 Acute water flea and fish toxicity

Acute aquatic data were sourced from the US EPA's ECOTOX database. Again, when more than one value was obtained for an active ingredient, the geometric mean was calculated. When measured data, suitable surrogates or other acceptable studies based on different exposure periods or species were unavailable to estimate ecotoxicity, Environment Canada's ESB was consulted for assistance with selecting the most appropriate QSAR for estimating *Daphnia magna* and fathead minnow toxicity. ESB expertise was sought since they had generated a number of *Daphnia magna* and fathead minnow toxicity estimates for DSL substances through application of various QSARs including, ECOWIN, TOPKAT, ASTER, OASIS and the Probablistic Neural Network (PNN).[4] Based on their knowledge of the training sets used to develop these QSARs, ESB staff selected the most appropriate QSAR for each NPRI substance lacking aquatic toxicity information.

### 3.1.5 Modifications to CHEMS toxicity parameters

The original CHEMS model included a chronic aquatic endpoint (*i.e.* fish NOEC) (Swanson *et al.* 1997). However, since fish NOECs were not readily available in the literature and the QSAR suggested by the model for estimating fish NOECs was a permutation of other data used in CHEMS (*i.e.* log $K_{OW}$ and 96-hour fish $LC_{50}$), the NOEC was not perceived to add value to the model and was excluded. For example, in the CHEMS risk ranking of the Toxic Release Inventory, all of the fish NOEC values were estimated using a QSAR based on 96-hour fish $LC_{50}$

[4] Explanation of each of these QSARs is provided by ESB's *Guidance Manual for the Categorization of Organic and Inorganic Substances on Canada's Domestic Substance List* (Environment Canada 2003).

and log $K_{OW}$. The original CHEMS model also included an acute terrestrial parameter represented by the rat oral $LD_{50}$ under environmental effects (Swanson *et al.* 1997). However, by including this endpoint twice in the model, the rat oral $LD_{50}$ was doubly weighted. For our purposes, this endpoint was removed and a new environmental effect parameter was added to the model (*i.e. Daphnia magna* $LC/EC_{50}$). Other environmental endpoints were explored for inclusion in the model; however, due to lack of available, consistent data, acute *Daphnia magna* toxicity was the only suitable endpoint that could be added to CHEMS.

## 3.2 Exposure Potential Data

Exposure data were sourced from Environment Canada's ESB (Gobas 2000) or estimated using QSARs or fugacity modelling.

### *3.2.1 Persistence*

In the most recent version of CHEMS, persistence is represented by water half-life determined by taking one over the sum of the inverse function of a substance's biological oxygen demand (BOD) half-life[5] and the inverse function of a substance's hydrolysis half-life (Swanson 2000a):

$$Water\ Half-life = \frac{1}{\left(\frac{1}{BOD} + \frac{1}{Hydrolysis}\right)}$$

However, after careful review of the water half-life equation, it was decided to replace this parameter with a more global estimate of environmental persistence. Since NPRI substances are released to all media and substances will move and partition to other media even if they are initially released to water, it seemed more reasonable for the persistence endpoint to include half-lives for air, soil, sediment and water. As such, an overall environmental half-life which incorporates half-lives for all environmental media was used to represent persistence in place of water half-life. Due to scarcity of reliable and comparable half-life data, persistence was estimated by fugacity modelling. The Level III model calculates three persistences, including persistence attributable to advection only ($T_A$), reaction only ($T_R$) and overall persistence ($T_O$). Overall persistence is a combination of advection and reaction and calculated as follows:

$$T_O = [1/T_A + 1/T_R]^{-1}$$

According to the model developers, global chemical persistence is best represented by reaction persistence, while local persistence is best represented by overall persistence (CEMC 2006). Advection can greatly diminish a substance's local concentration, without removing it permanently from the environment, and thereby reduce its overall half-life significantly. Considering Canada's large land area, a substance with high advection could be predicted to have very low overall persistence when in truth the chemical could be transported from one region in Canada to another where it could persist and potentially cause environmental effects. For example, fugacity modelling for dichloromethane predicts $T_R$ of 2380 hr, $T_A$ of 109 hr and $T_O$ of 105 hr. Since advection is rapid relative to reaction, the chemical is removed from the local environment but likely persists in another area since its reaction half-life is predicted to be in excess of 90 days. To prevent underestimating the hazard of substances with markedly reduced

[5] BOD half-life is the time required to biodegrade a chemical such that its BOD in water is reduced by 50%.

overall persistence due to rapid advection, the reaction half-life ($T_R$) was chosen to represent persistence over the overall half-life ($T_O$).

As explained in Appendix 1, the level III fugacity model has many data requirements, including environmental emission rates. The emission rates are normally defaulted to 1000 kg/h for each medium. However, since NPRI release data is available for each medium, the respective annual releases to each medium were used in place of the default emission rates to allow for a more accurate estimate of reaction half-life. This provides a more sophisticated estimate of reaction half-life since persistence can be affected by what medium the substance is introduced into and how it moves from one medium to another.

#### *3.2.2 Bioaccumulation/Bioconcentration*

Bioaccumulation and bioconcentration factors for fish were supplied by Environment Canada's ESB (Gobas 2000). Although bluegill sunfish (*Lepomis macrochirus*) is the preferred species for this measure, factors from different fish species were included due to scarcity of bioconcentration data. If measured values were not available from ESB, the bioconcentration factor was estimated by the following QSAR developed by Bintein *et al.* (1993):

$$log\ BCF = 0.910(\log K_{OW}) - 1.975\ \log[(6.8 \times 10^{-7})K_{OW} + 1] - 0.786$$

Log $K_{OW}$ values used in the QSAR were sourced from the Epiwin's PhysProp Database. When measured log $K_{OW}$ values were not available, they were estimated by Epiwin's KOWWIN QSAR.

## 4.0 HAZARD VALUES

Once the data was compiled, a hazard value (HV) was calculated for each parameter following the protocols outlined by Swanson *et al*. (1997). Transforming data to hazard values is an essential step in scoring systems as it normalizes all endpoints to the same relative scale and allows their further manipulation (e.g. addition, multiplication) by eliminating the complications of different units and varying magnitude. HVs ranged between 0 to 5 for effect parameters and 1 to 2.5 for persistence and bioconcentration factor. NPRI release amounts were transformed to release-weighting factors ranging between 1 and 10.

### 4.1 Converting Toxicity Values to Hazard Values

Toxicity endpoints were assigned HVs on a scale of 0 to 5 according to severity. A value of 0 represented negligible toxicity while a value of 5 indicated high toxicity. As discussed earlier, six endpoints were used to represent human health and environmental effects:

- rat oral $LD_{50}$;
- rat inhalation $LC_{50;}$
- carcinogenicity rating;
- reference dose/concentration (RfD/RfC);
- fish $LC_{50}$; and
- water flea $EC_{50}$

#### *4.1.1 Hazard values for acute rat oral and inhalation toxicity*

HVs for the oral $LD_{50}$ ($HV_{OR}$) and inhalation $LC_{50}$ ($HV_{INH}$) endpoints were calculated using a continuous, logarithmic-linear function. Cut-off values for the $LD_{50}$ were established based on

commonly accepted cut-off values (Swanson *et al.* 1997). The original cut-off values for the inhalation $LC_{50}$ were set at >10,000 ppm and <31.6 ppm for assigning HVs of 0 and 5, respectively. However, based on the Office of Prevention, Pesticides and Toxic Substances Guideline for acute inhalation toxicity (US EPA 1998) and the Pest Management Regulatory Agency (PMRA) cut-off values for pesticide labelling, these limit values appeared to be outdated. Therefore, new cut-off values, consistent with the PMRA's protocol for pesticide labelling, were established. Accordingly, the rat inhalation $LC_{50}$ cut-off values for setting HVs of 0 and 5 were > 2.0 mg/L and <0.05 mg/L, respectively. Table 2 illustrates the equations used to derive the HVs for the $LD_{50}$ and $LC_{50}$ endpoints. When no oral or inhalation toxicity information was available, a default hazard value of 2.5 was assigned to the chemical for that parameter.

**Table 2**: Equations used to derive hazard values from $LD_{50}$ oral and $LC_{50}$ inhalation data (Swanson *et al.* 1997)

| Acute Oral Toxicity ($HV_{OR}$) |
|---|
| If $LD_{50}$ oral > 5000 mg/kg, $HV_{OR} = 0$ |
| If $LD_{50}$ oral ≤ 5 mg/kg, $HV_{OR} = 5$ |
| For 5 mg/kg < $LD_{50}$ oral ≤ 5000 mg/kg, $HV_{OR} = 6.165 – 1.666 \log(LD_{50}\text{ oral})$ |

| 4-hour Acute Inhalation Toxicity ($HV_{INH}$) |
|---|
| If $LC_{50}$ inhalation > 2 mg/L, $HV_{INH} = 0$ |
| If $LC_{50}$ inhalation < 0.05 mg/L, $HV_{INH} = 5$ |
| For 0.05 mg/L ≤ $LC_{50}$ inhalation ≤ 2.0 mg/L $HV_{INH} = 0.9395 – 3.121 \log(LC_{50}\text{ inhalation})$ |

### *4.1.2 Hazard values for carcinogenicity ratings*

HVs for carcinogenicity ($HV_{CAR}$) were assigned based on the method shown in Table 3. When carcinogenicity ratings were not available from IARC or IRIS and information was lacking to categorize a chemical based on expert judgment, the substance was assigned a default value of 1.5 for $HV_{CAR}$ in accordance with recommendations made by Swanson and Socha (1997) regarding how to handle missing data in chemical ranking schemes. This default value (1.5) was chosen in place of the midpoint value (2.5) since 2.5 is not among the suite of carcinogenicity hazard values available (Table 3). Assigning a $HV_{CAR}$ of 1.5 instead of 2.5 when carcinogenicity data is lacking offers a degree of conservatism without unrealistically inflating the contribution to hazard from carcinogenicity.

**Table 3**: Carcinogenicity scoring based on IARC and US EPA classifications (Swanson *et al.* 1997)

| IARC classification | $HV_{CAR}$ | US EPA classification | $HV_{CAR}$ |
|---|---|---|---|
| Group 4 | 0 | Group E | 0 |
| Group 3 | 0 | Group D | 0 |
| Not Applicable (no IARC equivalent) | | Group C | 1.5 |
| Group 2B | 3.5 | Group B2 | 3.5 |
| Group 2A | 4.0 | Group B1 | 4.0 |
| Group 1 | 5.0 | Group A | 5.0 |

### *4.1.3 Hazard values for non-cancer effects*

HVs for non-cancer effects ($HV_{NCAR}$) were determined using the RfD or RfC. Upper and lower limits for the reference values were based on cut-offs provided by Swanson (2000a) for oral and inhalation NOAELs. Since the RfD and RfC are usually derived by dividing the NOAEL by a factor of 100, the cut-off values were also divided by a factor of 100. The equations shown in Table 4 were used to calculate $HV_{NCAR}$. When no information was available on which to base a reference value, a default hazard value of 2.5 was assigned to the chemical.

**Table 4**: Equations used to derive $HV_{NCAR}$ values from RfD or RfC (Swanson 2000a)

| Non-Cancer Toxicity ($HV_{NCAR}$) – Oral |
|---|
| If RfD > 10 mg/kg, $HV_{RfD} = 0$ |
| If RfD ≤ 0.001 mg/kg, $HV_{RfD} = 5$ |
| For 0.001 mg/kg ≤ RfD ≤ 10 mg/kg, |
| $HV_{RfD} = 1.25 – 1.25 \log(RfD)$ |

| Non-Cancer Toxicity ($HV_{NCAR}$) – Inhalation |
|---|
| If RfC > 30 mg/m$^3$, $HV_{RfC} = 0$ |
| If RfC < 0.003 mg/m$^3$, $HV_{RfC} = 5$ |
| For 0.003 mg/m$^3$ ≤ RfC ≤ 2.0 mg/L |
| $HV_{RfC} = 1.846 – 1.25 \log(RfC)$ |

#### *4.1.4 Hazard values for acute Daphnia and fish toxicity*

HVs for acute aquatic toxicity to fish ($HV_{AAF}$) and water flea ($HV_{AAD}$) were calculated using 96-hour fathead minnow (*Pimephales promelas*) $LC_{50}$ and 48-hour *Daphnia magna* $LC_{50}$ or $EC_{50}$ values, respectively, as illustrated in Table 5. A continuous, logarithmic-linear function was used to calculate both the $HV_{AAF}$ and $HV_{AAD}$ (Swanson *et al*. 1997). Commonly accepted cut-off values were chosen for the fish $LC_{50}$. The same cut-offs were applied to *Daphnia* $LC/EC_{50}$ values as supported by Snyder *et al*. (2000). When measured data or information on which to base *Daphnia* or fathead minnow toxicity were unavailable, a default hazard value of 2.5 was assigned to the chemical.

**Table 5**: Equations used to derive hazard values from fathead minnow $LC_{50}$ (Swanson *et al.* 1997) and *Daphnia magna* $LC/EC_{50}$ data (Snyder *et al.* 2000)

| Acute Aquatic Fish Toxicity ($HV_{AAF}$) |
|---|
| If $LC_{50} \geq 1000$ mg/L, $HV_{AAF} = 0$ |
| If $LC_{50} < 1$ mg/L, $HV_{AAF} = 5$ |
| For 1 mg/L ≤ $LC_{50}$ < 1000 mg/L, |
| $HV_{AAT} = -1.67 \log (LC_{50}) + 5.0$ |

| Acute Aquatic *Daphnia* Toxicity ($HV_{AAD}$) |
|---|
| If $LC/EC_{50} \geq 1000$ mg/L, $HV_{AAD} = 0$ |
| If $LC/EC_{50} < 1$ mg/L, $HV_{AAD} = 5$ |
| For 1 mg/L ≤ $LC/EC_{50}$ < 1000 mg/L, |
| $HV_{AAD} = - 1.67 \log (LC/EC_{50}) + 5.0$ |

### 4.2 Converting Exposure Data into Hazard Values

Exposure endpoints were assigned HVs on a scale of 1 to 2.5. A value of 1 represented negligible persistence and bioaccumulation potential while 2.5 indicated high persistence and high bioaccumulation potential. As discussed earlier, three endpoints were used as surrogates for exposure potential:

- reaction half-life (persistence);
- aquatic bioaccumulation/bioconcentration factor (BAF/BCF); and
- NPRI release amount (exposure potential and route of entry).

#### *4.2.1 Persistence and bioaccumulation/bioconcentration factor*

Persistence and BCFs were assigned HVs ranging from 1 to 2.5. As with the effect parameters, higher HVs for exposure parameters represented a higher level of hazard and lower HVs represented a lower level of hazard in terms of environmental fate.

Table 6 illustrates the criteria used to determine HVs for reaction half-life and aquatic bioconcentration. Calculations for the reaction half-life HV ($HV_{PERS}$) and aquatic bioaccumulation/bioconcentration HV ($HV_{BCF}$) were based on a continuous, logarithmic-linear scale to generate values between 1 and 2.5 (Swanson *et al*. 1997).

**Table 6**: Equations used to derive hazard values from Reaction half-life and Bioconcentration Factor (BCF) data (Swanson *et al*. 1997, Swanson 2000a)

| Reaction Half-life ($HV_{PERS}$) | Bioconcentration Factor ($HV_{BCF}$) |
|---|---|
| If Reaction $t_{1/2} \leq 4$ days, $HV_{PERS} = 1$ | If $\log(BAF/BCF) \leq 1.0$, $HV_{BCF} = 1$ |
| If Reaction $t_{1/2} > 500$ days, $HV_{PERS} = 2.5$ | If $\log(BAF/BCF) > 4.0$, $HV_{BCF} = 2.5$ |
| For 4 d < Reaction $t_{1/2} \leq 500$ d, | For $1.0 < \log(BAF/BCF) \leq 4.0$, |
| $HV_{PERS} = 0.311 \ln$ (Reaction $t_{1/2}$) + 0.568 | $HV_{BCF} = 0.5 \log(BAF/BCF) + 0.5$ |

### *4.2.2 NPRI environmental release amounts*

The NPRI environmental releases were not converted to hazard values like all the other parameters in the model. Instead, environmental releases reported to NPRI were converted to release-weighting factors (RWFs) on a scale of 1 to 10 (Table 7). Medium-specific RWFs were determined relative to the largest substance released in each medium. For example, ammonia was released to water in the largest quantity in the 2003 inventory. Therefore, ammonia's $RWF_{water}$ was assigned the highest factor, 10, and $RWF_{water}$ for all other substances were calculated relative to ammonia's releases to water. RWFs were calculated for air ($RWF_A$), water ($RWF_W$), land+water ($RWF_{LW}$) and total releases ($RWF_T$).

**Table 7**: Calculation of release weighting factors

$$RWF_m = \ln [\text{release amount } (kg)_m] + a$$

where

$$a = 10 - \ln [\text{maximum release amount } (kg)_m], \text{ and}$$

m = medium (water, air, land)

NPRI release data is reported under various categories as shown in Table 8. Therefore, to allow for reproducible risk ranking results, it is important to identify which categories were included to derive each RWF. For the purpose of calculating $RWF_A$, the release amount to air was determined by summing air releases from stacks, storage, fugitive, spills and other non-point sources.

**Table 8**: NPRI release, disposal and transfer categories (Environment Canada 2004)

| On-Site Releases | On-Site and Off-Site Disposal | Off-Site Transfers |
|---|---|---|
| **Air**<br>• stack/point<br>• storage/handling<br>• fugitive<br>• spills<br>• other non-point<br><br>**Surface Water**<br>• spills<br>• leaks<br>• direct discharge<br>**Land**<br>• spills<br>• leaks<br>• other | **Land**<br>• landfill containment<br>• land application or land farming<br>• underground injection<br>• storage (for off-site disposal only) | **Treatment**<br>• physical<br>• chemical<br>• biological<br>• incineration or thermal<br>• municipal sewage treatment plant (MSTP) |

In the case of $RWF_W$, total water releases were determined by adding surface water spills, leaks, direct discharges plus transfers to MSTPs. Transfers to MSTPs were incorporated in the total since few MSTPs are designed to handle industrial effluents so many organic substances enter and leave these systems unchanged. The $RWF_{LW}$ included all the categories included in $RWF_W$ plus the amounts released to land as spills, leaks and other and disposed to landfills and landfarms. Underground injection and storage were not included in calculation for releases to land and water since these types of disposals are contained and unlikely to contaminate the surrounding area. Finally, the $RWF_T$ was calculated by adding together all on-site releases, disposals to landfarm and landfill and discharges to MSTPs.

A method was developed to ensure that RWF values fell within a range from 1 to 10. By taking the natural logarithm of the release volume of each substance plus a constant (a), a normal distribution of data points was produced (Table 7). To ensure RWF values fell on a normalized scale from 1 to 10 representative of their release amounts, a cut-off value was established based on calculations shown in Table 9. Any release volume below this cut-off value was assigned a RWF of 1. This procedure ensured that release volumes less than the cut-off value would not produce a negative RWF or skew the resultant values.

**Table 9**: Calculation of Release Weighting Factor Cut-off Value

$RWF_m = 1$ for release amount (kg) < b

where

$b = e^{(1-a)}$

m = medium

## 5. 0 APPLYING THE CHEMS MODEL

Once all the toxicity, fate and environmental release data has been transformed into HVs or RWFs for a given set of chemicals, the CHEMS model has two applications. The HVs or the HVs and RWFs can be combined to generate a total hazard score (THS) or release-weighted risk score (RS), respectively, for each chemical. When the scores have been computed for each substance, they can be ranked accordingly in terms of hazard or risk.

### 5.1 Total Hazard Score

The CHEMS model compiles a total hazard score by multiplying the sum of effect HVs by the sum of exposure HVs as shown in Table 10.

**Table 10**: Modified CHEMS Total Hazard Score

| | |
|---|---|
| | Total Hazard Score (THS) = Effects $\times$ Exposure |
| Where: | Effects = $HV_{OR} + HV_{INH} + HV_{CAR} + HV_{NCAR} + HV_{AAF} + HV_{AAD}$ |
| | Exposure = $HV_{PERS} + HV_{BCF}$ |

For any given chemical, effects and exposure could have a maximum score of 30 and 5, respectively. Therefore, the maximum THS score for any given substance would be 150 (*i.e.* 5 x 30). A THS of 150 would indicate that a substance was extremely toxic, bioaccumulative and persistent in the environment. Conversely, a THS of 5 would indicate that a substance generally had low toxicity, persistence and bioaccumulation potential.

The THS gives an indication of a substance's hazard potential *if* it is present in the environment. *If* is emphasized in italics to underscore the fact that the total hazard score does not consider whether the chemical is present in the environment. Environmental presence is the single factor, aside from toxicity, which can have the greatest impact on increasing or diminishing a substance's risk to the environment or human health. However, since the THS does not incorporate environmental exposure, its use in prioritizing substances for risk assessment or management activities is limited to a theoretical scenario where all chemicals are released to the environment in the same quantity. The THS is the first step in characterizing a substance's hazard potential; incorporating environmental releases into the score gives a more accurate estimate of environmental risk and improves its utility for priority setting in the real world.

### 5.2 Risk Score

Clearly, to get a better perspective on the risk a chemical poses to the environment, environmental exposure must be included in the evaluation. The integration of toxicity, fate and environmental exposure data is made possible through the CHEMS risk score. While environmental releases reported to the NPRI are not equivalent to exposure concentrations, they nonetheless provide a good indicator of the relative presence of substances in the environment. Further, by combining environmental releases with toxicity, persistence and bioaccumulation data, the CHEMS risk score provides a reasonable proxy for risk.

As shown in Table 11, environmental releases are incorporated into the CHEMS model by multiplying the effect HVs by their corresponding RWF to yield release-weighted HVs (wHVs). The specific RWFs in Section 4.2.2 were calculated intentionally as they reflect the exposure pathways for each of the toxicity measures. For example, $HV_{INH}$ was multiplied by $RWF_A$ since inhalation exposure generally occurs through air. Similarly, the aquatic endpoints were multiplied by the $RWF_W$ since aquatic exposure to chemicals occurs via water. The chronic endpoints ($HV_{CAR}$ and $HV_{NCAR}$) were multiplied by $RWF_T$ since over a lifetime an individual can potentially be exposed to the total amount of the chemical deposited in the environment, regardless of its partitioning. Finally, $HV_{OR}$ was multiplied by $RWF_{LW}$ since oral exposures can result through ingestion of water and soil.

**Table 11**: Release Weighting Factors Multiplied by Effect Hazard Values (Swanson *et al.* 1997)

| | |
|---|---|
| $wHV_{OR} = HV_{OR} \times RWF_{LW}$ | where: |
| $wHV_{INH} = HV_{INH} \times RWF_A$ | $RWF_{LW}$ = land/water release weighting factor |
| $wHV_{CAR} = HV_{CAR} \times RWF_T$ | $RWF_A$ = air release weighting factor |
| $wHV_{NCAR} = HV_{NCAR} \times RWF_T$ | $RWF_T$ = total release weighting factor |
| $wHV_{AAF} = HV_{AAF} \times RWF_W$ | $RWF_W$ = water release weighting factor |
| $wHV_{AAD} = HV_{AAD} \times RWF_W$ | |

After each effect HV is multiplied by its corresponding RWF, a risk score (RS) is calculated by employing the paradigm "risk = effects x exposure". Similar to the total hazard score, the sum of wHVs is multiplied by the sum of exposure HVs to yield a risk score for each substance as shown in Table 12.

**Table 12**: The Modified CHEMS Risk Score

Risk Score (RS) = Release-Weighted Effects × Exposure

where: Release-Weighted Effects = $wHV_{OR} + wHV_{INH} + wHV_{CAR} + wHV_{NCAR} + wHV_{AAF} + wHV_{AAD}$

Exposure Potential = $HV_{PERS} + HV_{BCF}$

Once all of the risk scores have been tallied for a group of substances, they can then be ranked according to their respective risk scores.

## 5.3 Uncertainty Score

While not included in the original CHEMS model, an uncertainty score was calculated for each substance to place its total hazard and risk ranks within the context of its data gaps. In general, each toxicity and fate endpoint for each substance was assigned an uncertainty factor ranging from 0 to 4 depending on the source and reliability of the data. For example, *measured* data were assigned an uncertainty factor of zero while toxicity and fate data derived from expert judgment, QSARs or surrogates were assigned an uncertainty factor of two. A description of the rationale used to assign uncertainty factors for other data deficiencies is provided in Appendix 2. Once

uncertainty factors had been assigned for each endpoint, they were summed to yield an uncertainty score for each substance up to a maximum score of 28.

The primary purpose of the uncertainty score is to ground truth a substance's overall hazard or risk rank. For example, a chemical with a very low uncertainty score and high risk rank would endorse its addition to a priority list for future management. The low uncertainty score confirms that mostly measured data were used to establish the risk score; therefore, risk managers can be assured the risk posed by the substance is real and not an artefact of inflated hazard values due to missing or estimated data. Similarly, a substance with a low risk rank but high uncertainty score may support its addition to a priority list since further study (primarily testing) is required before it can be judged to present a low risk.

## 6.0 RESULTS AND DISCUSSION

The methodology outlined above was employed to yield national rankings based on hazard and risk scores as shown in Table 13. The rank according to volume of release is also provided for comparison. Lastly the uncertainty score has been provided to place a substance's risk and hazard ranks within the context of its data gaps. For simplicity, only the ordinal ranks are shown for risk, hazard and volume whereas the score is provided for uncertainty.

It is important to note that the risk rankings are relative because the RWFs used in the model are assigned relative to the largest environmental releases to each medium. In this way, the model only allows for a comparison of risk between the substances included in the ranking. Comparison of risk scores between risk rankings compiled for separate groups of chemicals is not possible.

**Table 13:** National Relative Rankings based on Risk, Hazard and Volume[6]

| Substance | Risk Rank | Hazard Rank | Volume Rank | Uncertainty Score |
|---|---|---|---|---|
| Ammonia | 1 | 36 | 1 | 6 |
| Hydrogen sulphide | 2 | 6 | 9 | 11 |
| Sulphuric acid | 3 | 26 | 5 | 10 |
| Chlorine | 4 | 19 | 25 | 11 |
| Benzene | 5 | 15 | 18 | 2 |
| Acrolein | 6 | 3 | 35 | 2 |
| Formaldehyde | 7 | 33 | 17 | 4 |
| Hydrochloric acid | 8 | 30 | 4 | 10 |
| Hydrogen fluoride | 9 | 43 | 11 | 9 |
| Phosphorus (yellow or white) | 10 | 2 | 73 | 10 |
| Nonylphenol | 11 | 13 | 37 | 7 |
| Naphthalene | 12 | 8 | 36 | 4 |
| Chlorine dioxide | 13 | 10 | 33 | 10 |
| Methylenebis (phenylisocyanate) | 14 | 5 | 41 | 9 |
| Phenol (and its salts) | 15 | 37 | 29 | 4 |
| Hydrogen cyanide | 16 | 1 | 56 | 10 |
| Sodium nitrite | 17 | 40 | 54 | 12 |
| Acetaldehyde | 18 | 45 | 20 | 4 |

[6] Complete scores and rankings are provided in Appendix 3.

| Substance | Risk Rank | Hazard Rank | Volume Rank | Uncertainty Score |
|---|---|---|---|---|
| Carbon disulphide | 19 | 16 | 10 | 12 |
| Nitric acid | 20 | 48 | 55 | 14 |
| Dichloromethane | 21 | 61 | 31 | 4 |
| Nitrate ion in solution at pH ≥ 6.0 | 22 | 76 | 2 | 12 |
| Hexane:n- | 23 | 32 | 8 | 8 |
| Xylene (mixed isomers) | 24 | 53 | 6 | 4 |
| Styrene | 25 | 49 | 13 | 4 |
| Biphenyl | 26 | 14 | 48 | 6 |
| Ethylbenzene | 27 | 46 | 21 | 4 |
| Calcium fluoride | 28 | 78 | 59 | 10 |
| Tetrachloroethylene | 29 | 12 | 53 | 2 |
| Trichloroethylene | 30 | 62 | 30 | 2 |
| Chloroform | 31 | 31 | 46 | 2 |
| Polymeric diphenylmethane diisocyanate | 32 | 22 | 47 | 9 |
| Sodium fluoride | 33 | 58 | 65 | 7 |
| Fluorine | 34 | 25 | 61 | 20 |
| Toluene | 35 | 77 | 7 | 2 |
| Trimethylbenzene:1,2,4- | 36 | 44 | 23 | 10 |
| Chloromethane | 37 | 69 | 32 | 8 |
| Methanol | 38 | 89 | 3 | 8 |
| Toluene-2,4-diisocyanate | 39 | 4 | 95 | 7 |
| Butadiene:1,3- | 40 | 55 | 45 | 8 |
| Cyanide ion | 41 | 9 | 75 | 6 |
| Vinyl acetate | 42 | 65 | 38 | 6 |
| Di-t-butyl-4-methylphenol:2,6- | 43 | 7 | 77 | 11 |
| Dichlorobenzene:p- | 44 | 18 | 63 | 4 |
| Cyclohexane | 45 | 68 | 19 | 8 |
| Butoxyethanol:2- | 46 | 83 | 26 | 12 |
| Acrylonitrile | 47 | 17 | 71 | 2 |
| Butyl benzyl phthalate | 48 | 21 | 64 | 2 |
| Ethylene oxide | 49 | 24 | 66 | 6 |
| Carbon tetrachloride | 50 | 11 | 89 | 2 |
| Bis(2-ethylhexyl) phthalate | 51 | 60 | 72 | 6 |
| Toluenediisocyanate (mixed isomers) | 52 | 20 | 79 | 7 |
| Methyl ethyl ketone | 53 | 92 | 12 | 8 |
| Triethylamine | 54 | 71 | 50 | 8 |
| Ethylene glycol | 55 | 95 | 15 | 9 |
| Isopropylidenediphenol:p,p'- | 56 | 23 | 70 | 9 |
| Anthracene | 57 | 27 | 68 | 8 |
| Vinyl chloride | 58 | 59 | 60 | 9 |
| Cresol (mixed isomers and their salts) | 59 | 63 | 52 | 8 |
| Isoprene | 60 | 38 | 67 | 8 |
| Hydroquinone (and its salts) | 61 | 28 | 97 | 7 |
| Acrylamide | 62 | 29 | 90 | 6 |
| Dibutyl phthalate | 63 | 34 | 74 | 2 |
| Cumene hydroperoxide | 64 | 35 | 96 | 15 |
| Cumene | 65 | 52 | 57 | 4 |
| Chlorobenzene | 66 | 39 | 86 | 2 |

| Substance | Risk Rank | Hazard Rank | Volume Rank | Uncertainty Score |
|---|---|---|---|---|
| Benzoyl peroxide | 67 | 41 | 99 | 12 |
| Bis(2-ethylhexyl) adipate | 68 | 42 | 78 | 5 |
| Diethanolamine (and its salts) | 69 | 81 | 51 | 7 |
| Methyl isobutyl ketone | 70 | 91 | 27 | 8 |
| Methyl-2-pyrrolidone:N- | 71 | 88 | 39 | 10 |
| Butyl alcohol:n- | 72 | 93 | 24 | 4 |
| Decabromodiphenyl oxide | 73 | 47 | 94 | 12 |
| Propylene | 74 | 82 | 22 | 11 |
| HCFC-141b | 75 | 66 | 44 | 14 |
| Ethylene | 76 | 84 | 16 | 11 |
| Lithium carbonate | 77 | 50 | 92 | 20 |
| Acrylic acid (and its salts) | 78 | 50 | 87 | 8 |
| Ethyl acrylate | 79 | 54 | 93 | 8 |
| Bromine | 80 | 56 | 85 | 14 |
| Butyl acrylate | 81 | 57 | 88 | 10 |
| Nitrilotriacetic acid (and its salts) | 82 | 67 | 81 | 14 |
| Dichloroethane:1,2- | 83 | 64 | 69 | 2 |
| Thiourea | 84 | 70 | 99 | 8 |
| HCFC-142b | 85 | 72 | 28 | 11 |
| Dicyclopentadiene | 86 | 73 | 76 | 8 |
| Phthalic anhydride | 87 | 74 | 91 | 13 |
| Isopropyl alcohol | 88 | 98 | 14 | 8 |
| Formic acid | 89 | 75 | 80 | 12 |
| Butyl alcohol:i- | 90 | 96 | 34 | 6 |
| Methyl methacrylate | 91 | 85 | 49 | 4 |
| Dioxane:1,4- | 92 | 79 | 84 | 8 |
| Maleic anhydride | 93 | 80 | 82 | 15 |
| Dimethylformamide:n,n- | 94 | 87 | 62 | 4 |
| Butyl alcohol:tert- | 95 | 94 | 58 | 8 |
| Methyl tert-butyl ether | 96 | 97 | 40 | 2 |
| HCFC-22 | 97 | 86 | 42 | 9 |
| Sulphur hexafluoride | 98 | 90 | 43 | 9 |
| Butyl alcohol:sec- | 99 | 99 | 83 | 8 |

The national risk rank demonstrates a shift in priorities when a chemical's fate and toxicity are considered in combination with its environmental releases. According to risk scores, the highest ranked substances include ammonia, hydrogen sulphide, sulphuric acid, chlorine, benzene, acrolein, formaldehyde, hydrochloric acid, hydrogen fluoride, and phosphorus. Following NPRI convention (*i.e.* ranking by volume), nitrate ion, n-hexane, xylene, toluene and methanol would have received national attention; however, they are deemed to be of lower priority given their low hazard.

Similarly, a different priority ranking would result if it was based on hazard alone. In contrast to the national risk rank, a priority ranking based on hazard would not include ammonia, sulphuric acid, formaldehyde, hydrochloric acid or hydrogen fluoride among its top ranks. Instead, it would include tetrachloroethylene, toluene-2,4-diisocyanate, cyanide ion, 2,6-dibutyl-4-methylphenol, p-dichlorobenzene, acrylonitrile and carbon tetrachloride – substances that all ranked much lower in terms of risk.

The risk rank also demonstrates a few risk principles through the rankings for ammonia and phosphorus. In spite of ammonia's medium rank for hazard, its high volume pushes ammonia into first place for risk. This outcome is expected considering, with the exception of four other chemicals, national ammonia releases are one to seven orders of magnitude greater than all other chemicals ranked. This demonstrates the following risk principle – a substance with moderate hazard can present a high risk to the environment if its environmental loading is high.

Conversely, in spite of the low volume rank for phosphorus, its high hazard rank raises its risk rank to eleventh highest, thereby illustrating that a substance with low environmental loading but high hazard can pose a high risk to the environment.

Clearly, the risk rank provides a superior prioritization of NPRI substances since it combines persistence, bioconcentration and toxicity data with NPRI release quantities. In spite of the clear cut ordering of risk suggested by the ordinal rank, the CHEMS risk ranking results should not be substituted for quantitative risk assessment nor used as an absolute for setting priorities. Rather, relative risk rankings generated by CHEMS should be used by risk managers as a tool for identifying priority substances for further evaluation.

To ground truth the risk ranking and ensure attention is focused on the most risky substances, the uncertainty score should be reviewed for each substance along with its relative risk rank. The uncertainty score helps substantiate a substance's overall rank and can also identify substances that require further study (*i.e.* those with high uncertainty scores). For example, a risk manager can be fairly certain that ammonia, benzene, formaldehyde and acrolein should be placed on a national priority list for further attention given their relatively low uncertainty scores. Similarly, the public can be assured that n-butyl alcohol, 1,2-dichloroethane and methyl methacrylate pose a low risk to the environment and human health since their low hazard and risk ranks are accompanied by low uncertainty scores. Finally, the moderate uncertainty scores for hydrogen sulphide, sulphuric acid, chlorine and hydrochloric acid suggest additional study or testing of these chemicals may be warranted to reduce the uncertainty of their respective risk ranks.

In addition to providing a national priority ranking, CHEMS can also be used to generate priority rankings for smaller geographical areas. To illustrate this concept, the relative risk rankings for Canada and a sample of its provinces are provided in Table 14[7].

[7] Relative risk, hazard and volume scores and ranks are provided for each province and territory in Appendices 4a-4l.

**Table 14**: National and Provincial Relative Risk Rankings

| | Risk Rank | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Substance** | **CA** | **NS** | **NB** | **ON** | **QC** | **SK** | **AB** | **BC** |
| Ammonia | 1 | 1 | 1 | 1 | 1 | 2 | 1 | 1 |
| Hydrogen sulphide | 2 | 2 | 3 | 4 | 4 | 1 | 2 | 2 |
| Sulphuric acid | 3 | 3 | 2 | 2 | 3 | 10 | 4 | 6 |
| Chlorine | 4 | 4 | 12 | 3 | 5 | 3 | 12 | 15 |
| Benzene | 5 | 7 | 9 | 7 | 8 | 4 | 3 | 10 |
| Chlorine dioxide | 6 | 20 | 7 | 11 | 2 | 5 | 15 | 3 |
| Acrolein | 7 | | 5 | 5 | 9 | | 8 | 19 |
| Formaldehyde | 8 | 10 | 4 | 17 | 6 | 14 | 9 | 4 |
| Hydrochloric acid | 9 | 6 | 11 | 6 | 13 | 12 | 11 | 7 |
| Hydrogen fluoride | 10 | | 13 | 12 | 7 | 6 | 7 | 5 |
| Phosphorus (yellow or white) | 11 | | | 9 | 29 | | 5 | 17 |
| Nonylphenol | 12 | | 6 | 8 | 20 | | 37 | 31 |
| Naphthalene | 13 | 8 | 20 | 16 | 17 | 7 | 6 | 22 |
| Methylenebis(phenylisocyanate) | 14 | | | 10 | 34 | | 16 | 11 |
| Phenol (and its salts) | 15 | 12 | 14 | 13 | 21 | 18 | 26 | 14 |
| Hydrogen cyanide | 16 | 5 | | 14 | | | | |
| Sodium nitrite | 17 | | | 15 | 14 | | 47 | 42 |
| Acetaldehyde | 18 | 9 | 8 | 22 | 11 | 9 | 18 | 8 |
| Biphenyl | 19 | 22 | | 29 | 43 | | 10 | 25 |
| Carbon disulphide | 20 | | | 31 | | 13 | 13 | 9 |
| Nitric acid | 21 | | 27 | 18 | 18 | 28 | 52 | 45 |
| Dichloromethane | 22 | | | 19 | 16 | | 24 | 13 |
| Hexane:n- | 23 | 13 | 15 | 21 | 24 | 11 | 14 | 18 |
| Calcium fluoride | 24 | | | 24 | 10 | 31 | 34 | 52 |
| Xylene (mixed isomers) | 25 | 19 | 19 | 20 | 28 | 8 | 21 | 21 |
| Styrene | 26 | 11 | | 28 | 19 | 15 | 20 | 12 |
| Nitrate ion | 27 | 15 | 16 | 23 | 26 | 16 | 19 | 16 |
| Ethylbenzene | 28 | 16 | 17 | 27 | 30 | 17 | 17 | 24 |
| Tetrachloroethylene | 29 | | | 32 | 12 | | 36 | 29 |
| Trichloroethylene | 30 | 14 | | 26 | 27 | | 55 | 34 |

A review of the rankings reveals that ammonia, hydrogen sulphide and sulphuric acid are the most common top ranking substances across the country. While top risk ranked substances are similar across the country, subtle differences exist between the provincial and national ranks (e.g. lower ranking for chlorine in NB, AB, BC, phosphorus in QC, formaldehyde in ON, SK, nonylphenol in AB, BC). The ranking differences highlight the power of CHEMS to identify priority substances for distinct geographical regions. Since the NPRI collects data on a per facility basis, it is possible to create relative risk rankings for very small areas. Presumably, given the different use and release patterns of chemicals throughout the country, unique priority lists could be developed for individual communities. Instead of being daunted by the entire, unwieldy NPRI list, the community-specific rankings would help Canadians glean more intelligible information from NPRI data and focus their efforts on reducing substances that present the most risk to their respective communities.

Whether used as a tool to set internal priorities within Environment Canada or to help Canadians navigate their way through the NPRI, the CHEMS risk ranking scheme is certainly an improvement from prioritizing and presenting NPRI substances in terms of total tonnes released.

## 7.0 LIMITATIONS AND UNCERTAINTIES

To make the overall risk rank more robust and reduce the uncertainty associated with the risk ranks, a data set comprised of mostly empirical data is desired. However, uncertainty from data deficiencies is inevitable when the CHEMS model, or any other risk ranking model for that matter, is applied to a large group of substances used in Canadian commerce. Although a great effort was made to collect measured data, and while the majority of data collected were measured (55%), many data deficiencies exist for NPRI substances. Consequently, as shown in Table 15, QSARs, expert judgment and default values were used to satisfy a number of endpoints in the CHEMS model. Most notably, the majority of BAF/BCFs and all persistence data (reaction $t_{1/2}$) were modelled.

**Table 15**: Percentage of measured, estimated and missing data points

| Endpoint | measured data (%) | estimated data[1] (%) | missing data[2] (%) |
|---|---|---|---|
| Rat oral $LD_{50}$ | 89 | 10 | 1 |
| Rat inhalation $LC_{50}$ | 67 | 33 | 0 |
| Carcinogenicity | 63 | 11 | 26 |
| Reference Dose/Concentration | 70 | 28 | 2 |
| *Daphnia* $EC_{50}$ | 67 | 30 | 3 |
| Fish $LC_{50}$ | 68 | 29 | 3 |
| Reaction $t_{1/2}$ | 0 | 100 | 0 |
| log $K_{OW}$ | 94 | 6 | 0 |
| BAF/BCF | 21 | 79 | 0 |

[1] Estimated by QSAR or expert judgement.
[2] Data requirement fulfilled by default value.

It is widely accepted that persistence and bioaccumulation data are scarce in the literature. For this reason, it's not surprising that a contract let by ESB (Gobas 2000) to locate bioaccumulation data only found BAF/BCFs for approximately 140 DSL substances – twenty-one of which were substances included in the NPRI risk rank. To overcome this glut of missing data, the bioconcentration potential was estimated by a QSAR relating log $K_{OW}$ to BCF. This practice is readily accepted by environmental fate experts when BCF data is unavailable (Environment Canada 2003) and helps diminish some of the uncertainty associated with estimated BCFs.

With respect to persistence, literature searches conducted by Environment Canada staff in headquarters and the Atlantic region yielded very few comparable half-life data for use in the NPRI risk ranking. However, most experts agree that the available models used for persistence prediction are fairly reliable (Robinson 2003). Therefore, due to scarcity of data and following expert recommendation, the fugacity model was chosen to estimate reaction half-lives for NPRI substances included in the risk rank.

Further, to shore up any uncertainty associated with choosing the most appropriate QSAR for the aquatic toxicity data gaps, ESB staff were consulted for expert opinion. Lastly, to counteract the uncertainty associated with using estimated and default values, an uncertainty score was calculated for each substance to balance its risk score with its data deficiencies. In this way, the uncertainty score helps identify data rich and data poor substances.

Measured data can also be a source of uncertainty if the test was not conducted according to good laboratory practice and erroneous toxicity values could result. To diminish uncertainty from outliers, the geometric or arithmetic mean was calculated when multiple values were available for an endpoint.

In large part, the CHEMS effect measures are derived from rat studies and acute exposures. As a result, the model could benefit from the inclusion of chronic aquatic and terrestrial studies. However, unless a significant amount of new data is generated, this suggestion is practically infeasible due to the paucity of these studies in the current literature. Further, including such effect measures in the CHEMS model would increase the overall uncertainty of the risk ranking since most chronic endpoints would likely be fulfilled by expert judgment, QSARs or default values.

The NPRI risk rank is also limited as it only encompasses a third of the NPRI substances and excludes substances with lower reporting thresholds (e.g. arsenic, lead, dioxins/furans, hexachlorobenzene, and polycyclic aromatic hydrocarbons). However, most of the latter substances have been extensively studied, have had a PSL assessment and/or been added to the CEPA list of toxic substances and are, therefore, being adequately managed by the government of Canada. A great deal of effort would be required to compile a comprehensive toxicity and fate database for all the organics and non-metallic inorganics on the NPRI. While this exercise is necessary to make the risk ranking applicable to all scenarios in Canada, it is uncertain what benefit would be derived from gathering such information. Given the criteria used to scale down the current risk rank (*i.e.* only substances with cumulative releases equivalent to or greater than 10 tonnes or reported by 5 or more facilities were included), it's unlikely that the national priority ranking would change even after a comprehensive database is compiled. For example, it is expected that substances more commonly reported or released in higher quantities would take precedence nationally over those substances released in very small quantities or reported by only a few facilities. With respect to metals, since the exposure endpoints in the CHEMS model are irrelevant for metals, a new ranking scheme needs to be developed to prioritize these substances.

A final uncertainty compromising the NPRI risk rank is the variability in the NPRI data itself. Since NPRI does not require polluters to measure their actual releases to the environment, a large portion of the inventory is estimated (*i.e.* based on mass balance, emission factors or engineering estimates). For this reason, the releases reported to the inventory have a certain amount of error associated with them. In addition, without resident experts on staff for each reporting sector and routine inspections to ensure consistent and complete reporting across all sectors, the inventory's comprehensiveness is in doubt. The NPRI is currently researching ways to improve the quality and comprehensiveness of NPRI data through data verification and on-site inspections. Therefore, program initiatives dedicated to improving reporting compliance and the inventory's data quality will help to reduce the uncertainty associated with NPRI release amounts in future NPRI risk ranking iterations.

## 8.0 RECOMMENDATIONS

- Ranking NPRI substances according to risk is a useful tool to assist priority setting within environmental and human health protection agencies and community groups with narrowing their focus on substances that present the greatest risk to their environment rather than those released in the greatest quantity.

- The CHEMS risk ranking model is a first step in identifying substances for further evaluation. Following higher tiers of risk assessment, risk managers can take action on substances earmarked by CHEMS, including the development of pollution reduction criteria, limiting the use of selected chemicals or perhaps instituting an economic instrument for those pollutants presenting the greatest environmental risk.

- There is some uncertainty associated with the risk scores due to data gaps being filled by modeling, expert judgment or default values and the uncertain reliability and comprehensiveness of reported NPRI data. Some of the uncertainty has been accounted for through the uncertainty score provided for each substance. Further, future program initiatives aimed at improving NPRI data quality should help reduce uncertainty from NPRI data.

- The work only encompasses a third of the NPRI substances and excludes metals. Therefore, a ranking system needs to be developed to prioritize metals on the NPRI; the current model is not appropriate since the exposure parameters (BAF/BCF, persistence) are not relevant to metals. While metals are beyond the scope of this report, a similar ranking system based on inherent toxicity and NPRI releases could be developed to prioritize metals on the NPRI. One obstacle to developing such a system is the absence of metal speciation information for metals reported to the NPRI. Currently the NPRI collects metal release data in the absence of parent compound information and thus the valence state of the metal is unknown. Without parent compound information, it is not possible to ascertain the bioavailability of reported metal releases. As such, until NPRI reporting is modified to collect this pertinent information, worst case scenario approaches would likely be used for assigning valence states, thereby adding uncertainty to the final ranking results.

- While the database is not comprehensive for all organics, it is a good start to help prioritize many of the substances on the NPRI. To make the tool applicable to all scenarios in Canada, a significant amount of time will be needed to collect toxicity and exposure data for the remaining NPRI substances. The benefit of expending resources on data collection for the remaining substances is questionable since the screening criteria used in the current risk rank should adequately address hazardous substances released in low quantities, provided they are commonly reported.

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## APPENDIX 1: FUGACITY MULTIMEDIA MODELS

The Level I, II and III fugacity models are based on the work of Mackay (1991). While each model becomes generally more sophisticated with increasing levels, each model attempts to provide a picture of how a chemical partitions in the environment. In all cases, model simulation requires the input of chemical and environmental properties.

In the Level I simulation, the volumes and densities of all 7 media (air, water, soil, bottom sediment, suspended sediment, fish and aerosols), organic carbon content of soil, sediment and suspended sediment, fish lipid content and physicochemical properties (water solubility, vapour pressure, log $K_{OW}$, melting point) must be supplied. While these criteria are required for input, it is possible to run any fugacity model by using the assumptions for volumes, densities, organic and fish lipid content provided by the model developers. The Level I model describes how a fixed quantity of conserved (non-reacting) chemical introduced into the environment partitions at equilibrium between the 7 media listed above. In this iteration there is no consideration of reaction.

The Level II model adds another level of sophistication by requiring reaction rates for all media and advective flow residence times for air, water and sediment burial. As opposed to introducing a fixed amount of chemical, the Level II model simulates a situation in which a chemical is continuously discharged at a constant rate and a steady-state is achieved in which input and output rates are equal. The medium receiving the emission is unimportant, because the chemical is assumed to become instantaneously distributed at equilibrium condition. In addition to providing environmental distribution of the chemical, by including advection and reaction rates, the Level II fugacity provides an estimate of chemical persistence and identifies which loss processes will be most important in removing a chemical from the environment.

The Level III simulation requires data on intermedia transport velocities and takes into account the movement of chemical from one medium to another in the calculation of environmental persistence. Unlike Level II, the Level III model does not assume equilibrium between media. This simulation provides a more realistic description of a chemical's fate including the important degradation and advection losses and the intermedia transport processes. The distribution of the chemical between media depends on how the chemical enters the system, (e.g. to air, water, or both) and the mode of entry affects the overall environmental persistence.

More information about fugacity modelling can be obtained from Mackay (1991).

## APPENDIX 2: RATIONALE FOR ASSIGNING UNCERTAINTY FACTORS

| Type of Uncertainty | Uncertainty Factor | N |
|---|---|---|
| Rat Oral $LD_{50}$ | | |
| Measured data | 0 | 88 |
| HV=0 based on expert judgement (*i.e.* ingestion unlikely) | 1 | 9 |
| Different species used | 2 | 1 |
| No information | 4 | 1 |
| Rat Inhalation $LC_{50}$ | | |
| Measured data | 0 | 66 |
| HV=0 based on expert judgement (*i.e.* inhalation irrelevant pathway) | 1 | 12 |
| Time-adjusted $LC_{50}$, surrogate chemical used or Green Seal equation | 2 | 20 |
| Time-adjusted and different species (mouse) | 3 | 1 |
| Carcinogenicity Rating | | |
| IARC or EPA evaluation | 0 | 62 |
| Surrogate or expert judgement based on supporting studies | 2 | 11 |
| No information | 4 | 26 |
| Reference Dose/ Reference Concentration | | |
| IRIS monograph or ATSDR Maximum Residue Limit | 0 | 69 |
| Expert judgement based on supporting studies, exposure limit | 2 | 28 |
| No information | 4 | 2 |
| *Daphnia magna* $EC/LC_{50}$ | | |
| Measured data | 0 | 66 |
| QSAR/surrogate/different exposure period/ $LC_{50}$> water solubility | 2 | 29 |
| QSAR-derived value of surrogate chemical | 3 | 1 |
| No information | 4 | 3 |
| Fathead minnow $LC_{50}$ | | |
| Measured data | 0 | 67 |
| QSAR/surrogate/different species/ $LC_{50}$> water solubility | 2 | 24 |
| QSAR & $LC_{50}$> water solubility/ QSAR-derived value from surrogate/ QSAR but ESB predicts high uncertainty | 3 | 5 |
| No information | 4 | 3 |
| BAF/BCF | | |
| measured data | 0 | 21 |
| QSAR based on measured log $K_{OW}$, expert judgement | 2 | 71 |
| QSAR based on modelled log $K_{OW}$ | 3 | 7 |
| Reaction half-life | | |
| Level III fugacity model | 2 | 99 |

## APPENDIX 3: CANADIAN RANKS AND SCORES

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 338.06 | 1 | 33.83 | 36 | 66463.318 | 1 | 6 |
| Hydrogen sulphide | 302.01 | 2 | 62.98 | 6 | 4871.019 | 9 | 11 |
| Sulphuric acid | 277.39 | 3 | 38.12 | 26 | 10636.701 | 5 | 10 |
| Chlorine | 244.46 | 4 | 45.53 | 19 | 824.913 | 25 | 11 |
| Benzene | 233.78 | 5 | 46.82 | 15 | 1703.912 | 18 | 2 |
| Acrolein | 191.91 | 6 | 69.50 | 3 | 305.38 | 35 | 2 |
| Formaldehyde | 189.36 | 7 | 34.87 | 33 | 1974.372 | 17 | 4 |
| Hydrochloric acid | 188.82 | 8 | 36.58 | 30 | 10751.557 | 4 | 10 |
| Hydrogen fluoride | 179.64 | 9 | 30.04 | 43 | 3785.693 | 11 | 9 |
| Phosphorus [1] | 178.26 | 10 | 73.66 | 2 | 8.105 | 73 | 10 |
| Nonylphenol | 168.77 | 11 | 47.13 | 13 | 177.098 | 37 | 7 |
| Naphthalene | 157.78 | 12 | 57.77 | 8 | 256.725 | 36 | 4 |
| Chlorine dioxide | 157.29 | 13 | 50.95 | 10 | 448.285 | 33 | 10 |
| Methylenebis (phenylisocyanate) | 148.28 | 14 | 65.22 | 5 | 105.084 | 41 | 9 |
| Phenol [2] | 142.83 | 15 | 33.59 | 37 | 733.441 | 29 | 4 |
| Hydrogen cyanide | 139.39 | 16 | 80.74 | 1 | 28.39 | 56 | 10 |
| Sodium nitrite | 130.45 | 17 | 32.13 | 40 | 38.575 | 54 | 12 |
| Acetaldehyde | 130.09 | 18 | 29.48 | 45 | 1246.53 | 20 | 4 |
| Carbon disulphide | 121.95 | 19 | 46.22 | 16 | 3825.992 | 10 | 12 |
| Nitric acid | 120.03 | 20 | 28.92 | 48 | 33.394 | 55 | 14 |
| Dichloromethane | 116.98 | 21 | 24.68 | 61 | 705.394 | 31 | 4 |
| Nitrate ion [3] | 115.12 | 22 | 18.58 | 76 | 42818.814 | 2 | 12 |
| Hexane:n- | 112.94 | 23 | 35.89 | 32 | 5978.501 | 8 | 8 |
| Xylene [4] | 108.30 | 24 | 26.78 | 53 | 7513.538 | 6 | 4 |
| Styrene | 104.18 | 25 | 28.20 | 49 | 2428.082 | 13 | 4 |
| Biphenyl | 94.26 | 26 | 47.03 | 14 | 66.601 | 48 | 6 |
| Ethylbenzene | 93.37 | 27 | 29.15 | 46 | 1148.335 | 21 | 4 |
| Calcium fluoride | 90.63 | 28 | 17.22 | 78 | 20.615 | 59 | 10 |
| Tetrachloroethylene | 87.46 | 29 | 48.08 | 12 | 41.871 | 53 | 2 |
| Trichloroethylene | 86.29 | 30 | 24.49 | 62 | 720.636 | 30 | 2 |
| Chloroform | 82.43 | 31 | 36.21 | 31 | 69.888 | 46 | 2 |
| Polymeric diphenylmethane diisocyanate | 80.71 | 32 | 40.48 | 22 | 66.963 | 47 | 9 |
| Sodium fluoride | 77.00 | 33 | 25.53 | 58 | 12.106 | 65 | 7 |
| Fluorine | 72.26 | 34 | 38.59 | 25 | 15.888 | 61 | 20 |
| Toluene | 71.60 | 35 | 18.40 | 77 | 6660.354 | 7 | 2 |
| Trimethylbenzene:1,2,4- | 69.82 | 36 | 29.55 | 44 | 957.588 | 23 | 10 |
| Chloromethane | 68.54 | 37 | 23.26 | 69 | 652.497 | 32 | 8 |
| Methanol | 67.18 | 38 | 7.51 | 89 | 23357.077 | 3 | 8 |
| Toluene-2,4-diisocyanate | 67.10 | 39 | 67.10 | 4 | 0.011 | 95 | 7 |
| Butadiene:1,3- | 65.26 | 40 | 26.24 | 55 | 77.491 | 45 | 8 |
| Cyanide ion | 63.99 | 41 | 57.62 | 9 | 6.149 | 75 | 6 |
| Vinyl acetate | 58.79 | 42 | 24.29 | 65 | 136.682 | 38 | 6 |
| Di-t-butyl-4-methylphenol:2,6- | 58.65 | 43 | 58.65 | 7 | 2.747 | 77 | 11 |
| Dichlorobenzene:p- | 56.76 | 44 | 45.66 | 18 | 13.037 | 63 | 4 |
| Cyclohexane | 56.33 | 45 | 23.47 | 68 | 1558.118 | 19 | 8 |

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Butoxyethanol:2- | 52.28 | 46 | 11.61 | 83 | 794.389 | 26 | 12 |
| Acrylonitrile | 50.48 | 47 | 46.01 | 17 | 8.601 | 71 | 2 |
| Butyl benzyl phthalate | 50.41 | 48 | 43.02 | 21 | 12.575 | 64 | 2 |
| Ethylene oxide | 50.12 | 49 | 39.50 | 24 | 11.875 | 66 | 6 |
| Carbon tetrachloride | 49.37 | 50 | 49.37 | 11 | 0.384 | 89 | 2 |
| Bis(2-ethylhexyl) phthalate | 46.51 | 51 | 24.87 | 60 | 8.217 | 72 | 6 |
| Toluenediisocyanate [4] | 44.69 | 52 | 44.69 | 20 | 1.586 | 79 | 7 |
| Methyl ethyl ketone | 44.21 | 53 | 6.86 | 92 | 3233.255 | 12 | 8 |
| Triethylamine | 42.85 | 54 | 22.45 | 71 | 48.065 | 50 | 8 |
| Ethylene glycol | 41.24 | 55 | 5.57 | 95 | 2323.543 | 15 | 9 |
| Isopropylidenediphenol:p,p'- | 40.22 | 56 | 40.22 | 23 | 8.77 | 70 | 9 |
| Anthracene | 39.36 | 57 | 37.56 | 27 | 10.218 | 68 | 8 |
| Vinyl chloride | 38.51 | 58 | 25.28 | 59 | 20.049 | 60 | 9 |
| Cresol [5] | 38.00 | 59 | 24.37 | 63 | 42.499 | 52 | 8 |
| Isoprene | 37.62 | 60 | 33.37 | 38 | 11.276 | 67 | 8 |
| Hydroquinone [2] | 37.48 | 61 | 37.48 | 28 | 0.002 | 97 | 7 |
| Acrylamide | 37.32 | 62 | 37.32 | 29 | 0.252 | 90 | 6 |
| Dibutyl phthalate | 34.58 | 63 | 34.58 | 34 | 6.779 | 74 | 2 |
| Cumene hydroperoxide | 34.23 | 64 | 34.23 | 35 | 0.007 | 96 | 15 |
| Cumene | 33.99 | 65 | 26.82 | 52 | 27.688 | 57 | 4 |
| Chlorobenzene | 33.20 | 66 | 33.20 | 39 | 0.608 | 86 | 2 |
| Benzoyl peroxide | 32.05 | 67 | 32.05 | 41 | 0 | 99 | 12 |
| Bis(2-ethylhexyl) adipate | 31.69 | 68 | 31.69 | 42 | 2.173 | 78 | 5 |
| Diethanolamine [2] | 31.26 | 69 | 13.75 | 81 | 47.22 | 51 | 7 |
| Methyl isobutyl ketone | 31.07 | 70 | 6.97 | 91 | 737.921 | 27 | 8 |
| Methyl-2-pyrrolidone:N- | 30.75 | 71 | 8.64 | 88 | 118.322 | 39 | 10 |
| Butyl alcohol:n- | 30.47 | 72 | 6.42 | 93 | 934.562 | 24 | 4 |
| Decabromodiphenyl oxide | 29.06 | 73 | 29.06 | 47 | 0.059 | 94 | 12 |
| Propylene | 28.22 | 74 | 12.67 | 82 | 1110.184 | 22 | 11 |
| HCFC-141b | 27.91 | 75 | 23.92 | 66 | 93.437 | 44 | 14 |
| Ethylene | 27.21 | 76 | 11.21 | 84 | 2188.485 | 16 | 11 |
| Lithium carbonate | 26.84 | 77 | 26.84 | 50 | 0.132 | 92 | 20 |
| Acrylic acid [2] | 26.84 | 77 | 26.84 | 50 | 0.561 | 87 | 8 |
| Ethyl acrylate | 26.57 | 79 | 26.57 | 54 | 0.114 | 93 | 8 |
| Bromine | 25.97 | 80 | 25.97 | 56 | 0.665 | 85 | 14 |
| Butyl acrylate | 25.75 | 81 | 25.75 | 57 | 0.386 | 88 | 10 |
| Nitrilotriacetic acid [2] | 24.99 | 82 | 23.81 | 67 | 1.31 | 81 | 14 |
| Dichloroethane:1,2- | 24.68 | 83 | 24.36 | 64 | 9.104 | 69 | 2 |
| Thiourea | 22.54 | 84 | 22.54 | 70 | 0 | 99 | 8 |
| HCFC-142b | 21.34 | 85 | 21.34 | 72 | 735.502 | 28 | 11 |
| Dicyclopentadiene | 20.79 | 86 | 20.79 | 73 | 3.713 | 76 | 8 |
| Phthalic anhydride | 20.29 | 87 | 20.29 | 74 | 0.211 | 91 | 13 |
| Isopropyl alcohol | 19.56 | 88 | 2.95 | 98 | 2339.335 | 14 | 8 |
| Formic acid | 19.23 | 89 | 19.23 | 75 | 1.571 | 80 | 12 |
| Butyl alcohol:i- | 18.02 | 90 | 4.61 | 96 | 316.567 | 34 | 6 |
| Methyl methacrylate | 16.90 | 91 | 9.79 | 85 | 50.177 | 49 | 4 |
| Dioxane:1,4- | 16.38 | 92 | 16.38 | 79 | 0.76 | 84 | 8 |

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Maleic anhydride | 14.75 | 93 | 14.75 | 80 | 1.116 | 82 | 15 |
| Dimethylformamide:n,n- | 12.69 | 94 | 9.04 | 87 | 13.748 | 62 | 4 |
| Butyl alcohol:tert- | 11.76 | 95 | 6.17 | 94 | 24.047 | 58 | 8 |
| Methyl tert-butyl ether | 11.50 | 96 | 4.60 | 97 | 107.23 | 40 | 2 |
| HCFC-22 | 9.13 | 97 | 9.13 | 86 | 104.957 | 42 | 9 |
| Sulphur hexafluoride | 7.01 | 98 | 7.01 | 90 | 95.079 | 43 | 9 |
| Butyl alcohol:sec- | 1.65 | 99 | 1.65 | 99 | 0.829 | 83 | 8 |

[1] yellow or white

[2] and its salts

[3] in solution at pH ≥ 6

[4] mixed isomers

[5] mixed isomers and their salts

## APPENDIX 4: PROVINCIAL AND TERRITORIAL RANKS AND SCORES

APPENDIX 4a: Relative Risk, Hazard and Volume Scores and Ranks for Nova Scotia

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 329.75 | 1 | 33.83 | 14 | 1234.703 | 2 | 6 |
| Hydrogen sulphide | 258.50 | 2 | 62.98 | 2 | 59.548 | 8 | 11 |
| Sulphuric acid | 239.32 | 3 | 38.12 | 8 | 981.652 | 3 | 10 |
| Chlorine | 226.86 | 4 | 45.53 | 7 | 40.68 | 10 | 11 |
| Hydrogen cyanide | 220.14 | 5 | 80.74 | 1 | 13.531 | 18 | 10 |
| Hydrochloric acid | 176.88 | 6 | 36.58 | 10 | 2038.986 | 1 | 10 |
| Benzene | 170.90 | 7 | 46.82 | 6 | 15.161 | 15 | 2 |
| Naphthalene | 122.52 | 8 | 57.77 | 3 | 0.779 | 27 | 4 |
| Acetaldehyde | 115.12 | 9 | 29.48 | 17 | 18.373 | 14 | 4 |
| Formaldehyde | 100.25 | 10 | 34.87 | 12 | 9.127 | 19 | 4 |
| Styrene | 97.96 | 11 | 28.20 | 19 | 46.72 | 9 | 4 |
| Phenol [1] | 92.46 | 12 | 33.59 | 15 | 1.199 | 26 | 4 |
| Hexane:n- | 91.40 | 13 | 35.89 | 11 | 27.265 | 11 | 8 |
| Nitrate ion [2] | 87.60 | 14 | 18.58 | 26 | 201.304 | 6 | 12 |
| Trichloroethylene | 81.03 | 15 | 24.49 | 22 | 14.1 | 17 | 2 |
| Ethylbenzene | 69.13 | 16 | 29.15 | 18 | 5.343 | 22 | 4 |
| Chloromethane | 65.95 | 17 | 23.26 | 25 | 14.3 | 16 | 8 |
| Methanol | 64.50 | 18 | 7.51 | 31 | 497.715 | 4 | 8 |
| Xylene [3] | 61.10 | 19 | 26.78 | 21 | 24.941 | 12 | 4 |
| Dibutyl phthalate | 56.42 | 20 | 34.58 | 13 | 5.03 | 23 | 2 |
| Chlorine dioxide | 50.95 | 21 | 50.95 | 4 | 0 | 33 | 10 |
| Trimethylbenzene:1,2,4- | 50.10 | 22 | 29.55 | 16 | 2.712 | 24 | 10 |
| Biphenyl | 47.03 | 23 | 47.03 | 5 | 0 | 33 | 6 |
| Ethylene glycol | 45.88 | 24 | 5.57 | 32 | 287.524 | 5 | 9 |
| Cyclohexane | 45.29 | 25 | 23.47 | 24 | 7.937 | 20 | 8 |
| Toluene | 43.47 | 26 | 18.40 | 27 | 18.563 | 13 | 2 |
| Anthracene | 37.56 | 27 | 37.56 | 9 | 0 | 33 | 8 |
| Cumene | 28.57 | 28 | 26.82 | 20 | 0.326 | 28 | 4 |
| Cresol [4] | 25.59 | 29 | 24.37 | 23 | 0.226 | 30 | 8 |
| Propylene | 23.19 | 30 | 12.67 | 29 | 6.545 | 21 | 11 |
| Isopropyl alcohol | 20.71 | 31 | 2.95 | 33 | 103.523 | 7 | 8 |
| Ethylene | 17.45 | 32 | 11.21 | 30 | 2.145 | 25 | 11 |
| Diethanolamine [1] | 13.75 | 33 | 13.75 | 28 | 0.245 | 29 | 7 |

[1] and its salts

[2] in solution at pH ≥ 6.0

[3] mixed isomers

[4] mixed isomers and their salts

APPENDIX 4b: Relative Risk, Hazard and Volume Scores and Ranks for New Brunswick

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 329.38 | 1 | 33.83 | 14 | 1071.541 | 3 | 6 |
| Sulphuric acid | 322.29 | 2 | 38.12 | 9 | 1622.277 | 2 | 10 |
| Hydrogen sulphide | 269.63 | 3 | 62.98 | 2 | 39.994 | 17 | 11 |
| Formaldehyde | 242.27 | 4 | 34.87 | 13 | 209.469 | 5 | 4 |
| Acrolein | 221.52 | 5 | 69.50 | 1 | 42.556 | 16 | 2 |
| Nonylphenol | 220.03 | 6 | 47.13 | 5 | 3.4 | 25 | 7 |
| Acetaldehyde | 192.73 | 7 | 29.48 | 18 | 153.489 | 7 | 4 |
| Benzene | 182.04 | 8 | 46.82 | 6 | 23.716 | 18 | 2 |
| Chloroform | 181.14 | 9 | 36.21 | 11 | 57.005 | 10 | 2 |
| Hydrochloric acid | 172.63 | 10 | 36.58 | 10 | 169.93 | 6 | 10 |
| Chlorine | 154.54 | 11 | 45.53 | 7 | 109.896 | 8 | 11 |
| Hydrogen fluoride | 152.33 | 12 | 30.04 | 16 | 52.09 | 12 | 9 |
| Chlorine dioxide | 142.42 | 13 | 50.95 | 4 | 50.719 | 13 | 10 |
| Phenol [1] | 120.12 | 14 | 33.59 | 15 | 55.596 | 11 | 4 |
| Hexane:n- | 97.25 | 15 | 35.89 | 12 | 48.47 | 14 | 8 |
| Nitrate ion [2] | 94.09 | 16 | 18.58 | 24 | 368.434 | 4 | 12 |
| Ethylbenzene | 82.55 | 17 | 29.15 | 19 | 16.188 | 19 | 4 |
| Methanol | 75.08 | 18 | 7.51 | 30 | 2207.058 | 1 | 8 |
| Xylene [3] | 65.16 | 19 | 26.78 | 21 | 46.645 | 15 | 4 |
| Naphthalene | 57.77 | 20 | 57.77 | 3 | 0 | 34 | 4 |
| Toluene | 51.00 | 21 | 18.40 | 25 | 73.54 | 9 | 2 |
| Cyclohexane | 48.75 | 22 | 23.47 | 23 | 14.869 | 20 | 8 |
| Trimethylbenzene:1,2,4- | 48.16 | 23 | 29.55 | 17 | 2.359 | 26 | 10 |
| Fluorine | 38.59 | 24 | 38.59 | 8 | 0 | 34 | 20 |
| Ethylene glycol | 37.94 | 25 | 5.57 | 32 | 1.033 | 27 | 9 |
| Methyl ethyl ketone | 30.50 | 26 | 6.86 | 31 | 11.611 | 21 | 8 |
| Nitric acid | 28.92 | 27 | 28.92 | 20 | 0 | 34 | 14 |
| Butadiene:1,3- | 26.24 | 28 | 26.24 | 22 | 0 | 34 | 8 |
| Propylene | 22.49 | 29 | 12.67 | 27 | 5.706 | 24 | 11 |
| Diethanolamine [1] | 13.75 | 30 | 13.75 | 26 | 0 | 34 | 7 |
| Methyl tert-butyl ether | 13.61 | 31 | 4.60 | 33 | 6.94 | 23 | 2 |
| Isopropyl alcohol | 13.59 | 32 | 2.95 | 34 | 10.025 | 22 | 8 |
| Ethylene | 11.21 | 33 | 11.21 | 28 | 0 | 34 | 11 |
| HCFC-22 | 9.13 | 34 | 9.13 | 29 | 0.856 | 28 | 9 |

[1] and its salts

[2] in solution at pH ≥ 6.0

[3] mixed isomers

APPENDIX 4c: Relative Risk, Hazard and Volume Scores and Ranks for Prince Edward Island

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 323.26 | 1 | 33.83 | 5 | 210.35 | 2 | 6 |
| Sulphuric acid | 153.38 | 2 | 38.12 | 2 | 16.8 | 4 | 10 |
| Hydrochloric acid | 153.17 | 3 | 36.58 | 3 | 43.99 | 3 | 10 |
| Nitrate ion [1] | 108.79 | 4 | 18.58 | 8 | 299.87 | 1 | 12 |
| Dichloromethane | 97.17 | 5 | 24.68 | 7 | 1.728 | 8 | 4 |
| Hexane:n- | 93.38 | 6 | 35.89 | 4 | 4.748 | 7 | 8 |
| Toluene | 53.66 | 7 | 18.40 | 9 | 15.8 | 5 | 2 |
| Methanol | 50.75 | 8 | 7.51 | 10 | 11.738 | 6 | 8 |
| Chlorine | 45.53 | 9 | 45.53 | 1 | 0 | 10 | 11 |
| Bromine | 25.97 | 10 | 25.97 | 6 | 0 | 10 | 14 |

[1] in solution at pH ≥ 6.0

APPENDIX 4d: Relative Risk, Hazard and Volume Scores and Ranks for Newfoundland and Labrador

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Benzene | 348.82 | 1 | 46.82 | 5 | 77.805 | 7 | 2 |
| Sulphuric acid | 331.49 | 2 | 38.12 | 7 | 353.64 | 3 | 10 |
| Ammonia | 313.57 | 3 | 33.83 | 9 | 443.002 | 2 | 6 |
| Acrolein | 268.63 | 4 | 69.50 | 1 | 48.961 | 14 | 2 |
| Chlorine | 243.79 | 5 | 45.53 | 6 | 15.25 | 16 | 11 |
| Hydrogen sulphide | 177.29 | 6 | 62.98 | 2 | 4.68 | 21 | 11 |
| Xylene [1] | 150.14 | 7 | 26.78 | 15 | 25.314 | 15 | 4 |
| Biphenyl | 144.22 | 8 | 47.03 | 4 | 11.846 | 18 | 6 |
| Acetaldehyde | 130.60 | 9 | 29.48 | 12 | 55.142 | 12 | 4 |
| Hexane:n- | 129.53 | 10 | 35.89 | 8 | 252.263 | 4 | 8 |
| Toluene | 123.89 | 11 | 18.40 | 17 | 64.311 | 11 | 2 |
| Ethylbenzene | 122.49 | 12 | 29.15 | 13 | 4.488 | 22 | 4 |
| Phenol [2] | 94.49 | 13 | 33.59 | 10 | 54.758 | 13 | 4 |
| Methanol | 75.08 | 14 | 7.51 | 19 | 752.759 | 1 | 8 |
| Cyclohexane | 67.11 | 15 | 23.47 | 16 | 72.235 | 8 | 8 |
| Trimethylbenzene:1,2,4- | 64.02 | 16 | 29.55 | 11 | 5.063 | 20 | 10 |
| Cyanide ion | 62.94 | 17 | 57.62 | 3 | 0.092 | 23 | 6 |
| Cumene | 58.07 | 18 | 26.82 | 14 | 12.568 | 17 | 4 |
| Diethanolamine [2] | 52.04 | 19 | 13.75 | 18 | 9.329 | 19 | 7 |
| Ethylene glycol | 47.60 | 20 | 5.57 | 22 | 162.394 | 5 | 9 |
| Methyl ethyl ketone | 45.84 | 21 | 6.86 | 21 | 67.08 | 9 | 8 |
| Methyl isobutyl ketone | 42.20 | 22 | 6.97 | 20 | 66.676 | 10 | 8 |
| Methyl tert-butyl ether | 24.03 | 23 | 4.60 | 23 | 99.835 | 6 | 2 |
| Isopropyl alcohol | 2.95 | 24 | 2.95 | 24 | 0.002 | 24 | 8 |

[1] mixed isomers

[2] and its salts

APPENDIX 4e: Relative Risk, Hazard and Volume Scores and Ranks for Quebec

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 336.34 | 1 | 33.83 | 31 | 9215.821 | 1 | 6 |
| Sulphuric acid | 273.42 | 2 | 38.12 | 22 | 759.525 | 8 | 10 |
| Hydrogen sulphide | 254.82 | 3 | 62.98 | 5 | 216.688 | 17 | 11 |
| Chlorine | 236.75 | 4 | 45.53 | 17 | 129.211 | 22 | 11 |
| Formaldehyde | 224.92 | 5 | 34.87 | 29 | 628 | 9 | 4 |
| Chlorine dioxide | 223.72 | 6 | 50.95 | 9 | 80.679 | 24 | 10 |
| Hydrogen fluoride | 201.63 | 7 | 30.04 | 38 | 1452.455 | 3 | 9 |
| Benzene | 159.50 | 8 | 46.82 | 14 | 44.963 | 30 | 2 |
| Acrolein | 150.34 | 9 | 69.50 | 2 | 11.65 | 44 | 2 |
| Acetaldehyde | 132.76 | 10 | 29.48 | 40 | 251.946 | 16 | 4 |
| Tetrachloroethylene | 130.60 | 11 | 48.08 | 11 | 29.356 | 35 | 2 |
| Hydrochloric acid | 130.48 | 12 | 36.58 | 26 | 403.075 | 11 | 10 |
| Sodium nitrite | 130.25 | 13 | 32.13 | 35 | 0 | 85 | 12 |
| Dichloromethane | 126.79 | 14 | 24.68 | 53 | 261.215 | 15 | 4 |
| Naphthalene | 125.98 | 15 | 57.77 | 7 | 3.664 | 53 | 4 |
| Nitric acid | 121.26 | 16 | 28.92 | 42 | 0.481 | 60 | 14 |
| Styrene | 120.43 | 17 | 28.20 | 43 | 1154.779 | 5 | 4 |
| Nonylphenol | 117.15 | 18 | 47.13 | 12 | 8.464 | 46 | 7 |
| Calcium fluoride | 113.45 | 19 | 17.22 | 68 | 7.245 | 47 | 10 |
| Phenol [1] | 108.35 | 20 | 33.59 | 32 | 164.132 | 21 | 4 |
| Fluorine | 106.21 | 21 | 38.59 | 21 | 15.6 | 38 | 20 |
| Sodium fluoride | 104.92 | 22 | 25.53 | 51 | 11.5 | 45 | 7 |
| Hexane:n- | 102.92 | 23 | 35.89 | 28 | 331.809 | 13 | 8 |
| Nitrate ion [2] | 93.75 | 24 | 18.58 | 66 | 1363.874 | 4 | 12 |
| Dichlorobenzene:p- | 92.13 | 25 | 45.66 | 16 | 13 | 40 | 4 |
| Chloroform | 88.70 | 26 | 36.21 | 27 | 12.057 | 42 | 2 |
| Trichloroethylene | 81.69 | 27 | 24.49 | 54 | 68.331 | 25 | 2 |
| Xylene [3] | 79.26 | 28 | 26.78 | 47 | 824.654 | 7 | 4 |
| Phosphorus [4] | 73.66 | 29 | 73.66 | 1 | 0 | 85 | 10 |
| Ethylbenzene | 72.13 | 30 | 29.15 | 41 | 27.539 | 36 | 4 |
| Methanol | 69.52 | 31 | 7.51 | 77 | 4081.275 | 2 | 8 |
| Toluene-2,4-diisocyanate | 67.10 | 32 | 67.10 | 3 | 0.002 | 77 | 7 |
| Methylenebis (phenylisocyanate) | 65.22 | 33 | 65.22 | 4 | 0.101 | 69 | 9 |
| Butyl benzyl phthalate | 63.81 | 34 | 43.02 | 19 | 12.467 | 41 | 2 |
| Trimethylbenzene:1,2,4- | 63.65 | 35 | 29.55 | 39 | 59.806 | 27 | 10 |
| Bis(2-ethylhexyl) phthalate | 63.57 | 36 | 24.87 | 52 | 6.147 | 48 | 6 |
| Bis(2-ethylhexyl) adipate | 59.23 | 37 | 31.69 | 37 | 0 | 85 | 5 |
| Di-t-butyl-4-methylphenol:2,6- | 58.65 | 38 | 58.65 | 6 | 0.145 | 66 | 11 |
| Toluene | 58.10 | 39 | 18.40 | 67 | 1057.345 | 6 | 2 |
| Cyanide ion | 57.62 | 40 | 57.62 | 8 | 0.294 | 61 | 6 |
| Acrylonitrile | 56.77 | 41 | 46.01 | 15 | 1.722 | 54 | 2 |
| Butadiene:1,3- | 53.85 | 42 | 26.24 | 49 | 5.341 | 50 | 8 |
| Carbon tetrachloride | 49.37 | 43 | 49.37 | 10 | 0.252 | 62 | 2 |
| Toluenediisocyanate [3] | 48.65 | 44 | 44.69 | 18 | 0.811 | 59 | 7 |
| Anthracene | 47.24 | 45 | 37.56 | 23 | 5.709 | 49 | 8 |
| Biphenyl | 47.03 | 46 | 47.03 | 13 | 0.071 | 72 | 6 |

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Cresol [5] | 46.06 | 47 | 24.37 | 55 | 13.84 | 39 | 8 |
| Ethylene glycol | 43.63 | 48 | 5.57 | 82 | 214.327 | 18 | 9 |
| Vinyl acetate | 43.15 | 49 | 24.29 | 56 | 5.117 | 51 | 6 |
| Methyl ethyl ketone | 41.20 | 50 | 6.86 | 80 | 265.257 | 14 | 8 |
| Polymeric diphenylmethane diisocyanate | 40.48 | 51 | 40.48 | 20 | 0.101 | 69 | 9 |
| Cyclohexane | 40.22 | 52 | 23.47 | 59 | 16.452 | 37 | 8 |
| Triethylamine | 37.53 | 53 | 22.45 | 61 | 4.02 | 52 | 8 |
| Hydroquinone [1] | 37.48 | 54 | 37.48 | 24 | 0 | 85 | 7 |
| Acrylamide | 37.32 | 55 | 37.32 | 25 | 0.146 | 65 | 6 |
| Dibutyl phthalate | 35.68 | 56 | 34.58 | 30 | 1.353 | 56 | 2 |
| Isoprene | 33.37 | 57 | 33.37 | 33 | 0.001 | 78 | 8 |
| Chlorobenzene | 33.20 | 58 | 33.20 | 34 | 0.083 | 71 | 2 |
| Benzoyl peroxide | 32.05 | 59 | 32.05 | 36 | 0 | 85 | 12 |
| HCFC-141b | 29.73 | 60 | 23.92 | 57 | 35.23 | 33 | 14 |
| Propylene | 29.44 | 61 | 12.67 | 70 | 210.055 | 19 | 11 |
| Butyl alcohol:n- | 29.07 | 62 | 6.42 | 81 | 40.029 | 32 | 4 |
| Dimethylformamide:n,n- | 29.05 | 63 | 9.04 | 75 | 11.958 | 43 | 4 |
| Methyl isobutyl ketone | 27.92 | 64 | 6.97 | 79 | 57.65 | 28 | 8 |
| Cumene | 27.25 | 65 | 26.82 | 46 | 1.244 | 57 | 4 |
| Lithium carbonate | 26.84 | 66 | 26.84 | 44 | 0.132 | 67 | 20 |
| Acrylic acid [1] | 26.84 | 66 | 26.84 | 44 | 0.16 | 64 | 8 |
| Ethyl acrylate | 26.57 | 68 | 26.57 | 48 | 0.022 | 73 | 8 |
| Ethylene | 26.16 | 69 | 11.21 | 72 | 197.496 | 20 | 11 |
| Butoxyethanol:2- | 25.94 | 70 | 11.61 | 71 | 43.763 | 31 | 12 |
| Butyl acrylate | 25.75 | 71 | 25.75 | 50 | 0.216 | 63 | 10 |
| Nitrilotriacetic acid [1] | 23.81 | 72 | 23.81 | 58 | 0.002 | 77 | 14 |
| Methyl methacrylate | 23.57 | 73 | 9.79 | 73 | 35.007 | 34 | 4 |
| Butyl alcohol:i- | 22.89 | 74 | 4.61 | 83 | 123.769 | 23 | 6 |
| Thiourea | 22.54 | 75 | 22.54 | 60 | 0 | 85 | 8 |
| HCFC-142b | 21.34 | 76 | 21.34 | 62 | 423.1 | 10 | 11 |
| Dicyclopentadiene | 20.79 | 77 | 20.79 | 63 | 0.006 | 75 | 8 |
| Isopropyl alcohol | 20.57 | 78 | 2.95 | 85 | 359.36 | 12 | 8 |
| Phthalic anhydride | 20.29 | 79 | 20.29 | 64 | 0.01 | 74 | 13 |
| Formic acid | 19.23 | 80 | 19.23 | 65 | 0.091 | 70 | 12 |
| Diethanolamine [1] | 16.82 | 81 | 13.75 | 69 | 1.683 | 55 | 7 |
| HCFC-22 | 9.13 | 82 | 9.13 | 74 | 64.8 | 26 | 9 |
| Methyl-2-pyrrolidone:N- | 8.64 | 83 | 8.64 | 76 | 0.979 | 58 | 10 |
| Sulphur hexafluoride | 7.01 | 84 | 7.01 | 78 | 50.53 | 29 | 9 |
| Methyl tert-butyl ether | 4.60 | 85 | 4.60 | 84 | 0 | 85 | 2 |

[1] and its salts

[2] in solution at pH ≥ 6.0

[3] mixed isomers

[4] yellow or white

[5] mixed isomers and their salts

APPENDIX 4f: Relative Risk, Hazard and Volume Scores and Ranks for Ontario

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 327.98 | 1 | 33.83 | 36 | 23265.171 | 2 | 6 |
| Sulphuric acid | 282.69 | 2 | 38.12 | 26 | 4950.662 | 5 | 10 |
| Chlorine | 256.54 | 3 | 45.53 | 19 | 454.659 | 24 | 11 |
| Hydrogen sulphide | 237.49 | 4 | 62.98 | 6 | 1380.286 | 11 | 11 |
| Acrolein | 208.04 | 5 | 69.50 | 3 | 151.708 | 33 | 2 |
| Hydrochloric acid | 198.39 | 6 | 36.58 | 30 | 5756.623 | 4 | 10 |
| Benzene | 196.67 | 7 | 46.82 | 15 | 499.709 | 23 | 2 |
| Nonylphenol | 192.92 | 8 | 47.13 | 13 | 165.205 | 31 | 7 |
| Phosphorus [1] | 192.86 | 9 | 73.66 | 2 | 8.102 | 58 | 10 |
| Methylenebis (phenylisocyanate) | 171.29 | 10 | 65.22 | 5 | 99.168 | 36 | 9 |
| Hydrogen fluoride | 162.63 | 11 | 30.04 | 43 | 623.244 | 17 | 9 |
| Phenol [2] | 153.27 | 12 | 33.59 | 37 | 121.395 | 35 | 4 |
| Hydrogen cyanide | 147.97 | 13 | 80.74 | 1 | 12.319 | 51 | 10 |
| Sodium nitrite | 145.36 | 14 | 32.13 | 40 | 37.288 | 43 | 12 |
| Naphthalene | 141.88 | 15 | 57.77 | 8 | 51.014 | 41 | 4 |
| Formaldehyde | 137.63 | 16 | 34.87 | 33 | 382.43 | 27 | 4 |
| Nitric acid | 131.11 | 17 | 28.92 | 48 | 32.818 | 47 | 14 |
| Dichloromethane | 122.03 | 18 | 24.68 | 60 | 298.179 | 28 | 4 |
| Xylene [3] | 115.24 | 19 | 26.78 | 52 | 4110.052 | 6 | 4 |
| Nitrate ion [4] | 114.74 | 20 | 18.58 | 74 | 25582.821 | 1 | 12 |
| Chlorine dioxide | 113.52 | 21 | 50.95 | 10 | 130.43 | 34 | 10 |
| Hexane:n- | 107.10 | 22 | 35.89 | 32 | 1488.744 | 10 | 8 |
| Acetaldehyde | 101.05 | 23 | 29.48 | 45 | 296.46 | 29 | 4 |
| Polymeric diphenylmethane diisocyanate | 97.24 | 24 | 40.48 | 22 | 64.951 | 38 | 9 |
| Trichloroethylene | 97.20 | 25 | 24.49 | 61 | 635.177 | 16 | 2 |
| Ethylbenzene | 96.15 | 26 | 29.15 | 46 | 584.874 | 20 | 4 |
| Styrene | 94.63 | 27 | 28.20 | 49 | 414.002 | 26 | 4 |
| Cyanide ion | 84.21 | 28 | 57.62 | 9 | 5.186 | 63 | 6 |
| Carbon disulphide | 81.15 | 29 | 46.22 | 16 | 59.6 | 39 | 12 |
| Tetrachloroethylene | 78.50 | 30 | 48.08 | 12 | 12.05 | 53 | 2 |
| Calcium fluoride | 77.53 | 31 | 17.22 | 76 | 10.299 | 55 | 10 |
| Chloromethane | 77.35 | 32 | 23.26 | 68 | 610.595 | 18 | 8 |
| Sodium fluoride | 76.15 | 33 | 25.53 | 57 | 0.606 | 76 | 7 |
| Trimethylbenzene:1,2,4- | 70.66 | 34 | 29.55 | 44 | 429.204 | 25 | 10 |
| Acrylonitrile | 67.58 | 35 | 46.01 | 17 | 6.829 | 60 | 2 |
| Toluene-2,4-diisocyanate | 67.10 | 36 | 67.10 | 4 | 0.009 | 89 | 7 |
| Butadiene:1,3- | 67.09 | 37 | 26.24 | 54 | 34.86 | 44 | 8 |
| Biphenyl | 65.37 | 38 | 47.03 | 14 | 8.928 | 56 | 6 |
| Methanol | 63.32 | 39 | 7.51 | 87 | 5960.507 | 3 | 8 |
| Ethylene oxide | 61.14 | 40 | 39.50 | 24 | 6.726 | 61 | 6 |
| Butoxyethanol:2- | 59.95 | 41 | 11.61 | 81 | 749.842 | 14 | 12 |
| Di-t-butyl-4-methylphenol:2,6- | 59.01 | 42 | 58.65 | 7 | 2.602 | 65 | 11 |
| Toluene | 58.12 | 43 | 18.40 | 75 | 3238.012 | 7 | 2 |
| Cyclohexane | 56.20 | 44 | 23.47 | 67 | 646.978 | 15 | 8 |
| Isoprene | 54.52 | 45 | 33.37 | 38 | 11.274 | 54 | 8 |

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Triethylamine | 53.62 | 46 | 22.45 | 69 | 33.417 | 46 | 8 |
| Isopropylidenediphenol:p,p'- | 53.41 | 47 | 40.22 | 23 | 8.765 | 57 | 9 |
| Butyl benzyl phthalate | 50.23 | 48 | 43.02 | 21 | 0.008 | 91 | 2 |
| Carbon tetrachloride | 49.37 | 49 | 49.37 | 11 | 0.001 | 95 | 2 |
| Methyl ethyl ketone | 48.27 | 50 | 6.86 | 90 | 2620.643 | 8 | 8 |
| Bis(2-ethylhexyl) phthalate | 47.39 | 51 | 24.87 | 59 | 2.07 | 66 | 6 |
| Dichlorobenzene:p- | 45.66 | 52 | 45.66 | 18 | 0.037 | 88 | 4 |
| Toluenediisocyanate [3] | 44.69 | 53 | 44.69 | 20 | 0.694 | 73 | 7 |
| Ethylene glycol | 42.09 | 54 | 5.57 | 93 | 1267.586 | 12 | 9 |
| Nitrilotriacetic acid [2] | 41.98 | 55 | 23.81 | 66 | 1.308 | 69 | 14 |
| Anthracene | 40.69 | 56 | 37.56 | 27 | 4.466 | 64 | 8 |
| Cresol [5] | 39.80 | 57 | 24.37 | 62 | 21.206 | 49 | 8 |
| Fluorine | 38.59 | 58 | 38.59 | 25 | 0.288 | 81 | 20 |
| Vinyl chloride | 38.47 | 59 | 25.28 | 58 | 8.064 | 59 | 9 |
| Hydroquinone [2] | 37.48 | 60 | 37.48 | 28 | 0.002 | 94 | 7 |
| Acrylamide | 37.32 | 61 | 37.32 | 29 | 0.106 | 85 | 6 |
| Chloroform | 36.21 | 62 | 36.21 | 31 | 0.006 | 93 | 2 |
| Chlorobenzene | 35.58 | 63 | 33.20 | 39 | 0.525 | 77 | 2 |
| Methyl isobutyl ketone | 34.83 | 64 | 6.97 | 89 | 558.09 | 22 | 8 |
| Decabromodiphenyl oxide | 34.63 | 65 | 29.06 | 47 | 0.059 | 87 | 12 |
| Dibutyl phthalate | 34.58 | 66 | 34.58 | 34 | 0.396 | 80 | 2 |
| Methyl-2-pyrrolidone:N- | 34.29 | 67 | 8.64 | 86 | 71.943 | 37 | 10 |
| Cumene hydroperoxide | 34.23 | 68 | 34.23 | 35 | 0.007 | 92 | 15 |
| Butyl alcohol:n- | 33.04 | 69 | 6.42 | 91 | 809.799 | 13 | 4 |
| Benzoyl peroxide | 32.05 | 70 | 32.05 | 41 | 0 | 97 | 12 |
| Vinyl acetate | 31.89 | 71 | 24.29 | 64 | 5.631 | 62 | 6 |
| Bis(2-ethylhexyl) adipate | 31.69 | 72 | 31.69 | 42 | 2.023 | 67 | 5 |
| Propylene | 29.05 | 73 | 12.67 | 80 | 583.062 | 21 | 11 |
| HCFC-141b | 28.63 | 74 | 23.92 | 65 | 58.207 | 40 | 14 |
| Acrylic acid [2] | 26.84 | 75 | 26.84 | 50 | 0.401 | 79 | 8 |
| Cumene | 26.82 | 76 | 26.82 | 51 | 1.894 | 68 | 4 |
| Ethyl acrylate | 26.57 | 77 | 26.57 | 53 | 0.092 | 86 | 8 |
| Ethylene | 26.02 | 78 | 11.21 | 82 | 590.418 | 19 | 11 |
| Bromine | 25.97 | 79 | 25.97 | 55 | 0.665 | 75 | 14 |
| Butyl acrylate | 25.75 | 80 | 25.75 | 56 | 0.164 | 83 | 10 |
| Dichloroethane:1,2- | 24.36 | 81 | 24.36 | 63 | 0.008 | 91 | 2 |
| Diethanolamine [2] | 23.78 | 82 | 13.75 | 79 | 12.177 | 52 | 7 |
| HCFC-142b | 21.34 | 83 | 21.34 | 70 | 205.706 | 30 | 11 |
| Isopropyl alcohol | 20.84 | 84 | 2.95 | 96 | 1526.83 | 9 | 8 |
| Dicyclopentadiene | 20.79 | 85 | 20.79 | 71 | 0.77 | 72 | 8 |
| Phthalic anhydride | 20.29 | 86 | 20.29 | 72 | 0.165 | 82 | 13 |
| Formic acid | 19.23 | 87 | 19.23 | 73 | 0.819 | 71 | 12 |
| Butyl alcohol:i- | 18.90 | 88 | 4.61 | 94 | 163.405 | 32 | 6 |
| Dioxane:1,4- | 16.38 | 89 | 16.38 | 77 | 0.438 | 78 | 8 |
| Methyl methacrylate | 16.03 | 90 | 9.79 | 83 | 15.152 | 50 | 4 |
| Butyl alcohol:tert- | 15.93 | 91 | 6.17 | 92 | 23.014 | 48 | 8 |
| Maleic anhydride | 14.75 | 92 | 14.75 | 78 | 1.088 | 70 | 15 |

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| HCFC-22 | 9.13 | 93 | 9.13 | 84 | 34.57 | 45 | 9 |
| Dimethylformamide:n,n- | 9.04 | 94 | 9.04 | 85 | 0.129 | 84 | 4 |
| Sulphur hexafluoride | 7.01 | 95 | 7.01 | 88 | 42.94 | 42 | 9 |
| Methyl tert-butyl ether | 4.60 | 96 | 4.60 | 95 | 0 | 97 | 2 |
| Butyl alcohol:sec- | 1.65 | 97 | 1.65 | 97 | 0.679 | 74 | 8 |

[1] yellow or white

[2] and its salts

[3] mixed isomers

[4] in solution at pH ≥ 6.0

[5] mixed isomers and their salts

APPENDIX 4g: Relative Risk, Hazard and Volume Scores and Ranks for Manitoba

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 338.33 | 1 | 33.83 | 13 | 3731.192 | 1 | 6 |
| Hydrogen sulphide | 220.12 | 2 | 62.98 | 2 | 103.189 | 7 | 11 |
| Sulphuric acid | 189.14 | 3 | 38.12 | 9 | 38.5 | 12 | 10 |
| Hexane:n- | 114.01 | 4 | 35.89 | 11 | 354.21 | 3 | 8 |
| Dichloromethane | 108.56 | 5 | 24.68 | 21 | 41.313 | 10 | 4 |
| Chlorine | 96.24 | 6 | 45.53 | 6 | 4.768 | 18 | 11 |
| Styrene | 93.70 | 7 | 28.20 | 18 | 54.012 | 9 | 4 |
| Acetaldehyde | 89.57 | 8 | 29.48 | 15 | 21.485 | 15 | 4 |
| Hydrochloric acid | 88.58 | 9 | 36.58 | 10 | 10.253 | 17 | 10 |
| Nitrate ion [1] | 83.81 | 10 | 18.58 | 25 | 219.018 | 5 | 12 |
| Benzene | 78.92 | 11 | 46.82 | 5 | 1.396 | 20 | 2 |
| Xylene [2] | 69.03 | 12 | 26.78 | 19 | 139.255 | 6 | 4 |
| Nitric acid | 65.95 | 13 | 28.92 | 17 | 0 | 39 | 14 |
| Methylenebis (phenylisocyanate) | 65.22 | 14 | 65.22 | 1 | 0.001 | 35 | 9 |
| Methanol | 64.92 | 15 | 7.51 | 32 | 1009.836 | 2 | 8 |
| Cyanide ion | 57.62 | 16 | 57.62 | 3 | 0.013 | 30 | 6 |
| Toluene | 56.31 | 17 | 18.40 | 26 | 325.257 | 4 | 2 |
| Ethylbenzene | 54.86 | 18 | 29.15 | 16 | 3.459 | 19 | 4 |
| Nonylphenol | 47.13 | 19 | 47.13 | 4 | 0 | 39 | 7 |
| Butyl benzyl phthalate | 43.02 | 20 | 43.02 | 7 | 0.1 | 28 | 2 |
| Polymeric diphenylmethane diisocyanate | 40.48 | 21 | 40.48 | 8 | 0 | 39 | 9 |
| Methyl ethyl ketone | 36.89 | 22 | 6.86 | 34 | 77.017 | 8 | 8 |
| Ethylene glycol | 35.35 | 23 | 5.57 | 36 | 36.1 | 13 | 9 |
| Formaldehyde | 34.87 | 24 | 34.87 | 12 | 0.299 | 23 | 4 |
| Trimethylbenzene:1,2,4- | 29.55 | 25 | 29.55 | 14 | 0.273 | 24 | 10 |
| Butyl alcohol:n- | 25.41 | 26 | 6.42 | 35 | 26.157 | 14 | 4 |
| Vinyl chloride | 25.28 | 27 | 25.28 | 20 | 0 | 39 | 9 |
| Trichloroethylene | 24.49 | 28 | 24.49 | 22 | 0.004 | 32 | 2 |
| Cyclohexane | 23.47 | 29 | 23.47 | 23 | 0.012 | 31 | 8 |
| Formic acid | 19.23 | 30 | 19.23 | 24 | 0.001 | 35 | 12 |
| Butyl alcohol:i- | 16.26 | 31 | 4.61 | 37 | 10.776 | 16 | 6 |
| Isopropyl alcohol | 16.02 | 32 | 2.95 |  | 40.515 | 11 | 8 |
| Diethanolamine [3] | 13.75 | 33 | 13.75 | 27 | 0.21 | 25 | 7 |
| Propylene | 12.67 | 34 | 12.67 | 28 | 0.014 | 29 | 11 |
| Butoxyethanol:2- | 11.61 | 35 | 11.61 | 29 | 0.156 | 26 | 12 |
| Ethylene | 11.21 | 36 | 11.21 | 30 | 0.001 | 35 | 11 |
| HCFC-22 | 9.13 | 37 | 9.13 | 31 | 0.149 | 27 | 9 |
| Methyl isobutyl ketone | 8.16 | 38 | 6.97 | 33 | 0.604 | 21 | 8 |
| Methyl tert-butyl ether | 4.60 | 39 | 4.60 | 38 | 0.455 | 22 | 2 |

[1] in solution at pH ≥ 6.0

[2] mixed isomers

[3] and its salts

APPENDIX 4h: Relative Risk, Hazard and Volume Scores and Ranks for Saskatchewan

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Hydrogen sulphide | 383.23 | 1 | 62.98 | 1 | 655.658 | 2 | 11 |
| Ammonia | 338.34 | 2 | 33.83 | 12 | 2445.559 | 1 | 6 |
| Chlorine | 260.04 | 3 | 45.53 | 7 | 29.711 | 15 | 11 |
| Benzene | 254.27 | 4 | 46.82 | 4 | 213.029 | 6 | 2 |
| Hydrogen fluoride | 160.67 | 5 | 30.04 | 15 | 73.8 | 10 | 9 |
| Naphthalene | 137.31 | 6 | 57.77 | 2 | 5.459 | 23 | 4 |
| Chlorine dioxide | 125.09 | 7 | 50.95 | 3 | 21.63 | 18 | 10 |
| Xylene [1] | 119.85 | 8 | 26.78 | 22 | 112.083 | 8 | 4 |
| Acetaldehyde | 118.27 | 9 | 29.48 | 17 | 16.477 | 20 | 4 |
| Sulphuric acid | 115.23 | 10 | 38.12 | 8 | 6.379 | 22 | 10 |
| Hexane:n- | 114.48 | 11 | 35.89 | 10 | 238.299 | 5 | 8 |
| Hydrochloric acid | 113.95 | 12 | 36.58 | 9 | 39.923 | 13 | 10 |
| Carbon disulphide | 113.51 | 13 | 46.22 | 5 | 67.8 | 11 | 12 |
| Formaldehyde | 109.54 | 14 | 34.87 | 11 | 16.384 | 21 | 4 |
| Styrene | 99.21 | 15 | 28.20 | 20 | 76.01 | 9 | 4 |
| Nitrate ion [2] | 94.90 | 16 | 18.58 | 26 | 368.82 | 4 | 12 |
| Ethylbenzene | 84.06 | 17 | 29.15 | 18 | 19.502 | 19 | 4 |
| Phenol [3] | 73.78 | 18 | 33.59 | 13 | 0.037 | 31 | 4 |
| Trimethylbenzene:1,2,4- | 66.26 | 19 | 29.55 | 16 | 22.116 | 17 | 10 |
| Methanol | 63.21 | 20 | 7.51 | 34 | 517.519 | 3 | 8 |
| Cyclohexane | 51.41 | 21 | 23.47 | 24 | 25.902 | 16 | 8 |
| Toluene | 48.66 | 22 | 18.40 | 27 | 56.186 | 12 | 2 |
| Acrylonitrile | 46.01 | 23 | 46.01 | 6 | 0.05 | 30 | 2 |
| Benzoyl peroxide | 32.05 | 24 | 32.05 | 14 | 0 | 40 | 12 |
| Ethylene glycol | 30.12 | 25 | 5.57 | 38 | 0.381 | 28 | 9 |
| Ethylene | 29.68 | 26 | 11.21 | 32 | 177.257 | 7 | 11 |
| Nitric acid | 28.92 | 27 | 28.92 | 19 | 0 | 40 | 14 |
| Propylene | 27.51 | 28 | 12.67 | 30 | 31.072 | 14 | 11 |
| Cumene | 26.82 | 29 | 26.82 | 21 | 0.036 | 32 | 4 |
| Bromine | 25.97 | 30 | 25.97 | 23 | 0 | 40 | 14 |
| Formic acid | 19.23 | 31 | 19.23 | 25 | 0 | 40 | 12 |
| Methyl isobutyl ketone | 17.39 | 32 | 6.97 | 35 | 2.187 | 24 | 8 |
| Calcium fluoride | 17.22 | 33 | 17.22 | 28 | 0.196 | 29 | 10 |
| Diethanolamine [3] | 13.75 | 34 | 13.75 | 29 | 0 | 40 | 7 |
| Methyl ethyl ketone | 13.44 | 35 | 6.86 | 36 | 0.95 | 25 | 8 |
| Butoxyethanol:2- | 13.19 | 36 | 11.61 | 31 | 0.468 | 27 | 12 |
| Butyl alcohol:n- | 11.41 | 37 | 6.42 | 37 | 0.893 | 26 | 4 |
| Methyl-2-pyrrolidone:N- | 8.64 | 38 | 8.64 | 33 | 0 | 40 | 10 |
| Butyl alcohol:i- | 4.61 | 39 | 4.61 | 39 | 0 | 40 | 6 |
| Isopropyl alcohol | 2.95 | 40 | 2.95 | 40 | 0 | 40 | 8 |

[1] mixed isomers

[2] in solution at pH ≥ 6.0

[3] and its salts

APPENDIX 4i: Relative Risk, Hazard and Volume Scores and Ranks for Alberta

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 312.37 | 1 | 33.83 | 25 | 11995.657 | 2 | 6 |
| Hydrogen sulphide | 277.25 | 2 | 62.98 | 4 | 1465.754 | 9 | 11 |
| Benzene | 235.33 | 3 | 46.82 | 12 | 791.623 | 12 | 2 |
| Sulphuric acid | 209.31 | 4 | 38.12 | 19 | 1767.929 | 7 | 10 |
| Phosphorus [1] | 208.50 | 5 | 73.66 | 1 | 0.002 | 63 | 10 |
| Naphthalene | 186.66 | 6 | 57.77 | 5 | 195.539 | 22 | 4 |
| Hydrogen fluoride | 183.02 | 7 | 30.04 | 30 | 1134.937 | 10 | 9 |
| Acrolein | 175.83 | 8 | 69.50 | 2 | 49.967 | 27 | 2 |
| Formaldehyde | 158.10 | 9 | 34.87 | 24 | 360.977 | 17 | 4 |
| Hydrochloric acid | 156.10 | 10 | 36.58 | 21 | 474.611 | 14 | 10 |
| Chlorine | 139.03 | 11 | 45.53 | 14 | 31.117 | 31 | 11 |
| Carbon disulphide | 136.00 | 12 | 46.22 | 13 | 2384.588 | 4 | 12 |
| Hexane:n- | 124.45 | 13 | 35.89 | 23 | 3194.761 | 3 | 8 |
| Nitrate ion [2] | 123.84 | 14 | 18.58 | 52 | 12937.484 | 1 | 12 |
| Biphenyl | 121.89 | 15 | 47.03 | 11 | 45.71 | 29 | 6 |
| Methylenebis (phenylisocyanate) | 115.70 | 16 | 65.22 | 3 | 0.104 | 57 | 9 |
| Ethylbenzene | 102.88 | 17 | 29.15 | 33 | 473.021 | 15 | 4 |
| Acetaldehyde | 102.20 | 18 | 29.48 | 32 | 179.95 | 23 | 4 |
| Chlorine dioxide | 87.95 | 19 | 50.95 | 7 | 15.099 | 36 | 10 |
| Styrene | 86.45 | 20 | 28.20 | 35 | 158.233 | 24 | 4 |
| Xylene [3] | 79.67 | 21 | 26.78 | 38 | 2115.797 | 6 | 4 |
| Vinyl acetate | 77.81 | 22 | 24.29 | 45 | 125.85 | 25 | 6 |
| Trimethylbenzene:1,2,4- | 76.73 | 23 | 29.55 | 31 | 433.713 | 16 | 10 |
| Dichloromethane | 76.64 | 24 | 24.68 | 41 | 28.661 | 32 | 4 |
| Fluorine | 74.51 | 25 | 38.59 | 18 | 0 | 70 | 20 |
| Phenol [4] | 71.95 | 26 | 33.59 | 26 | 300.072 | 19 | 4 |
| Ethylene oxide | 66.99 | 27 | 39.50 | 17 | 5.149 | 41 | 6 |
| Butadiene:1,3- | 64.81 | 28 | 26.24 | 39 | 15.335 | 35 | 8 |
| Methanol | 64.67 | 29 | 7.51 | 63 | 2249.891 | 5 | 8 |
| Cyclohexane | 62.20 | 30 | 23.47 | 47 | 767.26 | 13 | 8 |
| Toluene | 57.96 | 31 | 18.40 | 53 | 1561.795 | 8 | 2 |
| Cyanide ion | 57.62 | 32 | 57.62 | 6 | 0 | 70 | 6 |
| Vinyl chloride | 56.14 | 33 | 25.28 | 40 | 11.985 | 38 | 9 |
| Carbon tetrachloride | 49.37 | 34 | 49.37 | 8 | 0.131 | 54 | 2 |
| Tetrachloroethylene | 48.08 | 35 | 48.08 | 9 | 0.459 | 50 | 2 |
| Nonylphenol | 47.13 | 36 | 47.13 | 10 | 0.025 | 61 | 7 |
| Polymeric diphenylmethane diisocyanate | 45.97 | 37 | 40.48 | 16 | 1.911 | 45 | 9 |
| Dichloroethane:1,2- | 45.32 | 38 | 24.36 | 44 | 8.172 | 40 | 2 |
| Toluenediisocyanate [3] | 44.69 | 39 | 44.69 | 15 | 0.076 | 58 | 7 |
| Calcium fluoride | 42.98 | 40 | 17.22 | 54 | 2.815 | 43 | 10 |
| Diethanolamine [4] | 42.58 | 41 | 13.75 | 56 | 21.474 | 34 | 7 |
| Ethylene glycol | 40.66 | 42 | 5.57 | 68 | 318.416 | 18 | 9 |
| Cumene | 38.60 | 43 | 26.82 | 37 | 11.571 | 39 | 4 |
| Anthracene | 37.56 | 44 | 37.56 | 20 | 0.043 | 60 | 8 |
| Chloroform | 36.21 | 45 | 36.21 | 22 | 0.62 | 48 | 2 |

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Isoprene | 33.37 | 46 | 33.37 | 27 | 0.001 | 64 | 8 |
| Sodium nitrite | 32.13 | 47 | 32.13 | 28 | 0 | 70 | 12 |
| Bis(2-ethylhexyl) adipate | 31.69 | 48 | 31.69 | 29 | 0.15 | 53 | 5 |
| Methyl ethyl ketone | 31.14 | 49 | 6.86 | 65 | 41.808 | 30 | 8 |
| Ethylene | 29.91 | 50 | 11.21 | 59 | 1120.768 | 11 | 11 |
| Nitric acid | 28.92 | 51 | 28.92 | 34 | 0.05 | 59 | 14 |
| Propylene | 27.99 | 52 | 12.67 | 57 | 210.411 | 20 | 11 |
| Acrylic acid [4] | 26.84 | 53 | 26.84 | 36 | 0 | 70 | 8 |
| Trichloroethylene | 24.49 | 54 | 24.49 | 42 | 0.024 | 62 | 2 |
| Cresol [5] | 24.37 | 55 | 24.37 | 43 | 0.105 | 56 | 8 |
| Nitrilotriacetic acid [4] | 23.81 | 56 | 23.81 | 46 | 0 | 70 | 14 |
| Triethylamine | 22.45 | 57 | 22.45 | 48 | 0.568 | 49 | 8 |
| Dicyclopentadiene | 22.35 | 58 | 20.79 | 50 | 2.789 | 44 | 8 |
| Butyl alcohol:n- | 21.96 | 59 | 6.42 | 66 | 47.812 | 28 | 4 |
| HCFC-142b | 21.34 | 60 | 21.34 | 49 | 106.696 | 26 | 11 |
| Methyl isobutyl ketone | 20.74 | 61 | 6.97 | 64 | 23.856 | 33 | 8 |
| Formic acid | 19.23 | 62 | 19.23 | 51 | 0.66 | 47 | 12 |
| Isopropyl alcohol | 17.09 | 63 | 2.95 | 70 | 202.251 | 21 | 8 |
| Dioxane:1,4- | 16.38 | 64 | 16.38 | 55 | 0.322 | 51 | 8 |
| Butyl alcohol:i- | 11.93 | 65 | 4.61 | 69 | 12.804 | 37 | 6 |
| Butoxyethanol:2- | 11.61 | 66 | 11.61 | 58 | 0.117 | 55 | 12 |
| HCFC-22 | 9.13 | 67 | 9.13 | 60 | 3.886 | 42 | 9 |
| Dimethylformamide:n,n- | 9.04 | 68 | 9.04 | 61 | 1.661 | 46 | 4 |
| Methyl-2-pyrrolidone:N- | 8.64 | 69 | 8.64 | 62 | 0 | 70 | 10 |
| Butyl alcohol:tert- | 6.66 | 70 | 6.17 | 67 | 0.243 | 52 | 8 |

[1] yellow or white

[2] in solution at pH ≥ 6.0

[3] mixed isomers

[4] and its salts

[5] mixed isomers and their salts

APPENDIX 4j: Relative Risk, Hazard and Volume Scores and Ranks for British Columbia

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 336.06 | 1 | 33.83 | 24 | 12815.684 | 1 | 6 |
| Hydrogen sulphide | 333.17 | 2 | 62.98 | 4 | 945.222 | 6 | 11 |
| Formaldehyde | 183.40 | 3 | 34.87 | 23 | 367.686 | 9 | 4 |
| Hydrogen fluoride | 166.66 | 4 | 30.04 | 27 | 449.167 | 8 | 9 |
| Sulphuric acid | 152.30 | 5 | 38.12 | 18 | 139.337 | 14 | 10 |
| Hydrochloric acid | 148.76 | 6 | 36.58 | 20 | 1814.166 | 3 | 10 |
| Acetaldehyde | 136.57 | 7 | 29.48 | 29 | 253.208 | 10 | 4 |
| Chlorine dioxide | 130.46 | 8 | 50.95 | 7 | 149.728 | 12 | 10 |
| Carbon disulphide | 130.23 | 9 | 46.22 | 12 | 1314.004 | 5 | 12 |
| Benzene | 120.76 | 10 | 46.82 | 11 | 18.322 | 23 | 2 |
| Methylenebis (phenylisocyanate) | 107.11 | 11 | 65.22 | 3 | 5.71 | 32 | 9 |
| Styrene | 103.13 | 12 | 28.20 | 32 | 524.326 | 7 | 4 |
| Dichloromethane | 97.15 | 13 | 24.68 | 38 | 74.298 | 17 | 4 |
| Phenol [1] | 91.28 | 14 | 33.59 | 25 | 36.252 | 19 | 4 |
| Nitrate ion [2] | 87.95 | 15 | 18.58 | 50 | 1477.189 | 4 | 12 |
| Chlorine | 85.59 | 16 | 45.53 | 13 | 9.621 | 27 | 11 |
| Phosphorus [3] | 73.66 | 17 | 73.66 | 1 | 0.001 | 64 | 10 |
| Hexane:n- | 72.24 | 18 | 35.89 | 22 | 34.285 | 20 | 8 |
| Acrolein | 69.50 | 19 | 69.50 | 2 | 0.538 | 44 | 2 |
| Methanol | 69.41 | 20 | 7.51 | 61 | 6065.044 | 2 | 8 |
| Xylene [4] | 58.64 | 21 | 26.78 | 35 | 113.834 | 15 | 4 |
| Naphthalene | 57.77 | 22 | 57.77 | 5 | 0.27 | 45 | 4 |
| Cyanide ion | 57.62 | 23 | 57.62 | 6 | 0.133 | 49 | 6 |
| Ethylbenzene | 57.57 | 24 | 29.15 | 30 | 13.904 | 24 | 4 |
| Chloromethane | 53.40 | 25 | 23.26 | 45 | 27.602 | 22 | 8 |
| Butadiene:1,3- | 50.59 | 26 | 26.24 | 36 | 6.112 | 29 | 8 |
| Tetrachloroethylene | 48.08 | 27 | 48.08 | 8 | 0.006 | 60 | 2 |
| Toluene | 47.81 | 28 | 18.40 | 51 | 248.902 | 11 | 2 |
| Nonylphenol | 47.13 | 29 | 47.13 | 9 | 0.004 | 63 | 7 |
| Biphenyl | 47.03 | 30 | 47.03 | 10 | 0.046 | 53 | 6 |
| Triethylamine | 44.86 | 31 | 22.45 | 46 | 10.06 | 25 | 8 |
| Toluenediisocyanate [4] | 44.69 | 32 | 44.69 | 14 | 0.005 | 62 | 7 |
| Trichloroethylene | 41.74 | 33 | 24.49 | 39 | 3 | 34 | 2 |
| Polymeric diphenylmethane diisocyanate | 40.48 | 34 | 40.48 | 15 | 0 | 70 | 9 |
| Isopropylidenediphenol:p,p'- | 40.22 | 35 | 40.22 | 16 | 0.005 | 62 | 9 |
| Ethylene oxide | 39.50 | 36 | 39.50 | 17 | 0 | 70 | 6 |
| Anthracene | 37.56 | 37 | 37.56 | 19 | 0 | 70 | 8 |
| Cresol [5] | 37.48 | 38 | 24.37 | 40 | 7.122 | 28 | 8 |
| Methyl-2-pyrrolidone:N- | 37.14 | 39 | 8.64 | 60 | 45.4 | 18 | 10 |
| Chloroform | 36.21 | 40 | 36.21 | 21 | 0.2 | 46 | 2 |
| Methyl ethyl ketone | 33.73 | 41 | 6.86 | 64 | 148.889 | 13 | 8 |
| Sodium nitrite | 32.13 | 42 | 32.13 | 26 | 1.287 | 40 | 12 |
| Trimethylbenzene:1,2,4- | 31.68 | 43 | 29.55 | 28 | 2.04 | 37 | 10 |
| Cyclohexane | 31.65 | 44 | 23.47 | 44 | 5.814 | 30 | 8 |
| Nitric acid | 28.92 | 45 | 28.92 | 31 | 0.045 | 54 | 14 |

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Lithium carbonate | 26.84 | 46 | 26.84 | 33 | 0 | 70 | 20 |
| Cumene | 26.82 | 47 | 26.82 | 34 | 0.049 | 52 | 4 |
| Butyl acrylate | 25.75 | 48 | 25.75 | 37 | 0.006 | 60 | 10 |
| Dichloroethane:1,2- | 24.36 | 49 | 24.36 | 41 | 0.924 | 41 | 2 |
| Vinyl acetate | 24.29 | 50 | 24.29 | 42 | 0.084 | 50 | 6 |
| Nitrilotriacetic acid [1] | 23.81 | 51 | 23.81 | 43 | 0 | 70 | 14 |
| Methyl isobutyl ketone | 22.49 | 52 | 6.97 | 63 | 28.858 | 21 | 8 |
| Dicyclopentadiene | 20.79 | 53 | 20.79 | 47 | 0.148 | 48 | 8 |
| Phthalic anhydride | 20.29 | 54 | 20.29 | 48 | 0.036 | 56 | 13 |
| Formic acid | 19.23 | 55 | 19.23 | 49 | 0 | 70 | 12 |
| Ethylene glycol | 17.26 | 56 | 5.57 | 67 | 1.445 | 39 | 9 |
| Calcium fluoride | 17.22 | 57 | 17.22 | 52 | 0.06 | 51 | 10 |
| Diethanolamine [1] | 16.05 | 58 | 13.75 | 54 | 2.102 | 36 | 7 |
| Propylene | 15.81 | 59 | 12.67 | 55 | 4.213 | 33 | 11 |
| Butyl alcohol:n- | 15.10 | 60 | 6.42 | 65 | 9.872 | 26 | 4 |
| Isopropyl alcohol | 15.07 | 61 | 2.95 | 69 | 96.829 | 16 | 8 |
| Maleic anhydride | 14.75 | 62 | 14.75 | 53 | 0.028 | 57 | 15 |
| Ethylene | 12.28 | 63 | 11.21 | 57 | 2.304 | 35 | 11 |
| Butoxyethanol:2- | 11.61 | 64 | 11.61 | 56 | 0.043 | 55 | 12 |
| Methyl methacrylate | 9.79 | 65 | 9.79 | 58 | 0.018 | 58 | 4 |
| Butyl alcohol:i- | 9.47 | 66 | 4.61 | 68 | 5.813 | 31 | 6 |
| HCFC-22 | 9.13 | 67 | 9.13 | 59 | 0.696 | 43 | 9 |
| Sulphur hexafluoride | 7.01 | 68 | 7.01 | 62 | 1.609 | 38 | 9 |
| Butyl alcohol:tert- | 6.17 | 69 | 6.17 | 66 | 0.79 | 42 | 8 |
| Butyl alcohol:sec- | 1.65 | 70 | 1.65 | 70 | 0.15 | 47 | 8 |

[1] and its salts

[2] in solution at pH ≥ 6.0

[3] yellow or white

[4] mixed isomers

[5] mixed isomers and their salts

APPENDIX 4k: Relative Risk, Hazard and Volume Scores and Ranks for Nunavut

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 295.74 | 1 | 33.83 | 1 | 0.778 | 2 | 6 |
| Ethylene glycol | 55.74 | 2 | 5.57 | 2 | 33.84 | 1 | 9 |

APPENDIX 4l: Relative Risk, Hazard and Volume Scores and Ranks for Northwest Territories

| Substance | Risk Score | Risk Rank | Hazard Score | Hazard Rank | Total Release (tonnes) | Volume Rank | UF total |
|---|---|---|---|---|---|---|---|
| Ammonia | 318.22 | 1 | 33.83 | 6 | 33.86 | 3 | 6 |
| Benzene | 268.24 | 2 | 46.82 | 4 | 18.188 | 4 | 2 |
| Hydrogen cyanide | 267.77 | 3 | 80.74 | 1 | 2.54 | 8 | 10 |
| Cyanide ion | 255.98 | 4 | 57.62 | 3 | 0.431 | 13 | 6 |
| Butadiene:1,3- | 156.22 | 5 | 26.24 | 10 | 15.843 | 5 | 8 |
| Hexane:n- | 103.49 | 6 | 35.89 | 5 | 3.647 | 7 | 8 |
| Hydrogen sulphide | 62.98 | 7 | 62.98 | 2 | 0 | 16 | 11 |
| Xylene [1] | 59.43 | 8 | 26.78 | 9 | 0.963 | 9 | 4 |
| Trimethylbenzene:1,2,4- | 57.28 | 9 | 29.55 | 7 | 0.302 | 14 | 10 |
| Methanol | 50.54 | 10 | 7.51 | 15 | 3.735 | 6 | 8 |
| Cyclohexane | 48.74 | 11 | 23.47 | 11 | 0.659 | 10 | 8 |
| Toluene | 41.53 | 12 | 18.40 | 12 | 0.643 | 11 | 2 |
| Propylene | 40.07 | 13 | 12.67 | 13 | 59.106 | 2 | 11 |
| Ethylene | 37.42 | 14 | 11.21 | 14 | 98.096 | 1 | 11 |
| Ethylbenzene | 33.58 | 15 | 29.15 | 8 | 0.017 | 15 | 4 |
| Ethylene glycol | 26.28 | 16 | 5.57 | 16 | 0.497 | 12 | 9 |

[1] mixed isomers

## APPENDIX 5: RAW DATA AND REFERENCES

Information included in these tables is derived from 18 major references; these are cited throughout by the following abbreviations:

**ASTER:** QSAR used by ESB to predict aquatic toxicity for substances on the DSL for the purpose of categorization. See Appendix 5 of ESB's *Guidance Manual for the Categorization of Organic and Inorganic Substances on Canada's DSL* (Environment Canada 2003) for description of ASTER.

**Calculated:** As estimated from log $K_{OW}$ based on the equation: log BCF = 0.91 * log $K_{OW}$ - 1.975 * log(6.8e-07 * $K_{OW}$ + 1.0) - 0.786 [Bintein 1993].

**CESARS:** Chemical Evaluation Search and Retrieval System, Canadian Centre for Occupational Health and Safety (CCOHS). Available: http://www.ccohs.ca/. Retrieval 2003-2006.

**CHEMINFO:** Chemical Profiles Created by CCOHS. Available: http://www.ccohs.ca/. Retrieval 2003-2006.

**CHRIS:** Chemical Hazards Response Information System, CCOHS. Available: http://www.ccohs.ca/. Retrieval 2003-2006.

**ECOTOX:** ECOTOXicology Database System, U.S. Environmental Protection Agency. Available: http://www.epa.gov/ecotox/. Retrieval 2003-2006.

**ECOSAR:** QSAR used by ESB for estimating inherent toxicity of substances on DSL. See Appendix 5 of categorization manual (Environment Canada 2003) for description of ECOSAR.

**EHC:** Environmental Health Criteria Monographs, International Programme on Chemical Safety. Available: http://www.inchem.org/. Retrieval 2003-2006.

**Green Seal:** 2005. Green Seal standard GS-37: Environmental Standard for General-Purpose, Bathroom, Glass, and Carpet Cleaners Used for Industrial and Institutional Purposes (2nd edition). March 2005. Green Seal, Inc.

**HSDB:** Hazardous Substances Data Bank, United States National Library of Medicine. Available: http://toxnet.nlm.nih.gov/. Retrieval 2003-2006.

**IARC:** International Agency for Research on Cancer, World Health Organization. Available: http://www.iarc.fr/. Retrieval 2003-2006.

**IRIS:** Integrated Risk Information System, U.S. Environmental Protection Agency. Available: http://www.epa.gov/iris/. Retrieval 2003-2006.

**IUCLID:** International Uniform ChemicaL Information Database, European Chemicals Bureau. Available: http://ecb.jrc.it/esis/. Retrieval 2003-2006.

**KOWWIN:** QSAR available through EPI Suite v3.12 that provides log $K_{OW}$ estimates. Available through EPI Suite software downloadable from: http://www.epa.gov/oppt/exposure/docs/episuitedl.htm.

**OASIS:** QSAR used by ESB for estimating inherent toxicity of substances on DSL. See Appendix 5 of categorization manual (Environment Canada 2003) for description of OASIS.

**PhysProp:** Physical-chemical property database available through EPI Suite v3.12. Available: http://www.epa.gov/oppt/exposure/docs/episuitedl.htm. Retrieval 2003-2006.

**PNN:** Probablistic Neural Network. QSAR used by ESB for estimating inherent toxicity of substances on DSL. See Appendix 5 of categorization manual (Environment Canada 2003) for description of PNN.

**TOPKAT:** QSAR used by ESB for estimating inherent toxicity of substances on DSL. See Appendix 5 of categorization manual (Environment Canada 2003) for description of TOPKAT.

**Rat Oral $LD_{50}$**

| Chemical | $LD_{50}$ (mg/kg) | $LD_{50}$ range | N | Reference(s) | $UF_{OR}$ |
|---|---|---|---|---|---|
| Acetaldehyde | 1008 | 640 - 1930 | 5 | 1) CESARS<br>2) HSDB<br>3) EHC 167, 1995 | 0 |
| Acrolein | 44 | 42 - 46 | 2 | 1) CHEMINFO<br>2) CESARS<br>3) EHC 127, 1991 | 0 |
| Acrylamide | 168 | 124 - 203 | 5 | 1) CHEMINFO<br>2) CESARS | 0 |
| Acrylic acid [1] | 170 | 33.5 - 360 | 4 | 1) CHEMINFO<br>2) CESARS<br>3) EHC 191, 1997 | 0 |
| Acrylonitrile | 92 | 72 - 186 | 14 | 1) CESARS<br>2) CHEMINFO<br>3) EHC 28, 1983 | 0 |
| Ammonia | 350 | | 1 | HSDB | 0 |
| Anthracene | 16000 | | 1 | 1) IUCLID | 0 |
| Benzene | 3098 | 810 - 10032 | 13 | 1) CHEMINFO<br>2) HSDB<br>3) CESARS | 0 |
| Benzoyl peroxide | 7710 | | 1 | HSDB | 0 |
| Biphenyl | 3655 | 2400 - 5040 | 4 | 1) CHEMINFO<br>2) IUCLID | 0 |
| Bis(2-ethylhexyl) adipate | 7143 | 5600 - 9110 | 2 | HSDB | 0 |
| Bis(2-ethylhexyl) phthalate | 20011 | 6860 - 30600 | 5 | 1) CESARS<br>2) HSDB | 0 |
| Bromine | 2600 | | 1 | IUCLID | 0 |
| Butadiene:1,3- | 5480 | | 1 | 1) HSDB<br>2) IUCLID | 0 |
| Butoxyethanol:2- | 1110 | 470 - 3000 | 8 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |

| Chemical | $LD_{50}$ (mg/kg) | $LD_{50}$ range | N | Reference(s) | $UF_{OR}$ |
|---|---|---|---|---|---|
| Butyl acrylate | 2534 | 500 - 8053 | 8 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |
| Butyl alcohol:i- | 2762 | 2460 - 3100 | 2 | HSDB | 0 |
| Butyl alcohol:n- | 1588 | 790 - 2510 | 3 | 1) HSDB<br>2) CHEMINFO | 0 |
| Butyl alcohol:sec- | 6480 | | 1 | HSDB | 0 |
| Butyl alcohol:tert- | 3077 | 2733 - 3500 | 3 | 1) HSDB<br>2) IUCLID | 0 |
| Butyl benzyl phthalate | 7782 | 2330 - 16500 | 5 | 1) HSDB<br>2) CESARS | 0 |
| Calcium fluoride | 4250 | | 1 | HSDB | 0 |
| Carbon disulphide | 988 | 100 - 3188 | 4 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |
| Carbon tetrachloride | 5135 | 2800 - 23432 | 14 | 1) HSDB<br>2) EHC 208, 1999<br>3) CESARS | 0 |
| Chlorine | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely pathway as chlorine is gas at room temperature. | 1 |
| Chlorine dioxide | 292 | | 1 | CESARS | 0 |
| Chlorobenzene | 2644 | 1427 - 4000 | 5 | 1) HSDB<br>2) EHC 128,1991<br>3) CESARS<br>4) CHEMINFO | 0 |
| Chloroform | 1060 | 445.5 - 2180 | 9 | 1) HSDB<br>2) EHC 163, 1994<br>3) CESARS | 0 |
| Chloromethane | 1800 | | 1 | HSDB | 0 |
| Cresol [2] | 1454 | | 1 | CHEMINFO | 0 |
| Cumene | 2605 | 1400 - 5000 | 4 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |

| Chemical | $LD_{50}$ (mg/kg) | $LD_{50}$ range | N | Reference(s) | $UF_{OR}$ |
|---|---|---|---|---|---|
| Cumene hydroperoxide | 458 | 382 - 550 | 2 | 1) CHRIS<br>2) IUCLID | 0 |
| Cyanide ion | 8.4 | 3.4 - 26 | 5 | CESARS | 0 |
| Cyclohexane | 29820 | | 1 | HSDB | 0 |
| Decabromodiphenyl oxide | >5000 | | 1 | IUCLID | 0 |
| Dibutyl phthalate | 14201 | 8000 - 20000 | 3 | 1) HSDB<br>2) EHC 189, 1997<br>3) CESARS | 0 |
| Dichlorobenzene:p- | 2071 | 500 - 3863 | 4 | 1) HSDB<br>2) CESARS | 0 |
| Dichloroethane:1,2- | 854 | 670 - 1308 | 8 | 1) HSDB<br>2) EHC 176, 1995<br>3) CESARS | 0 |
| Dichloromethane | 2115 | 1410 - 3048 | 12 | 1) HSDB<br>2) EHC 164, 1996<br>3) CESARS | 0 |
| Dicyclopentadiene | 493 | 346.5 - 820 | 6 | 1) HSDB<br>2) CHRIS<br>3) IUCLID | 0 |
| Diethanolamine [1] | 1771 | 710 - 3450 | 13 | 1) HSDB<br>2) CHRIS<br>3) IUCLID | 0 |
| Dimethylformamide:n,n- | 3815 | 2200 - 7550 | 12 | 1) HSDB<br>2) EHC 114, 1991<br>3) IUCLID | 0 |
| Dioxane:1,4- | 5518 | 4200 - 7120 | 6 | 1) CESARS<br>2) CHEMINFO | 0 |
| Di-t-butyl-4-methylphenol:2,6- | 1832 | 890 - 2450 | 8 | 1) HSDB<br>2) CESARS<br>3) IUCLID | 0 |
| Ethyl acrylate | 1461 | 193 - 14800 | 11 | 1) HSDB<br>2) CESARS<br>3) EHC 191, 1997 | 0 |

| Chemical | $LD_{50}$ (mg/kg) | $LD_{50}$ range | N | Reference(s) | $UF_{OR}$ |
|---|---|---|---|---|---|
| Ethylbenzene | 4309 | 3500 - 5460 | 5 | 1) HSDB<br>2) EHC 186, 1996<br>3) CESARS | 0 |
| Ethylene | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely pathway as medium of concern is air and all NPRI releases are to air. | 1 |
| Ethylene glycol | 7502 | 4000 - 15280 | 22 | 1) HSDB<br>2) CESARS<br>3) IUCLID | 0 |
| Ethylene oxide | 323 | 280 - 365 | 3 | 1) HSDB<br>2) PSL Assessment 2001<br>2) EHC 55, 1985 | 0 |
| Fluorine | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely pathway as fluorine is a gas at room temperature. Soluble in water with decomposition forming HF. Medium of concern is air. | 1 |
| Formaldehyde | 283 | 100 - 800 | 2 | HSDB | 0 |
| Formic acid | 1402 | 730 - 3050 | 5 | 1) HSDB<br>2) CESARS<br>3) IUCLID | 0 |
| HCFC-141b | >5000 | | 1 | HSDB | 0 |
| HCFC-142b | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely pathway as HCFC-142b is a gas at room temperature and medium of concern is air. | 1 |
| HCFC-22 | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely pathway as HCFC-22 is a gas at room temperature and medium of concern is air. | 1 |
| Hexane:n- | 25057 | 15800 - 32400 | 7 | 1) HSDB<br>2) EHC 122, 1991<br>3) CESARS | 0 |
| Hydrochloric acid | 700 | | 1 | 1) IUCLID | 0 |
| Hydrogen cyanide | 4.1 | 3.62 - 4.5 | 3 | 1) IUCLID | 0 |

| Chemical | $LD_{50}$ (mg/kg) | $LD_{50}$ range | N | Reference(s) | $UF_{OR}$ |
|---|---|---|---|---|---|
| Hydrogen fluoride | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely since gas at room temperature, medium of concern is air and NPRI distribution is 100% to air. | 1 |
| Hydrogen sulphide | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely since gas at room temperature and medium of concern is air. | 1 |
| Hydroquinone [1] | 554 | 302 - 1080 | 7 | 1) HSDB<br>2) CHEMINFO<br>3) IUCLID | 0 |
| Isoprene | 2125 | 2043 - 2210 | 2 | IUCLID | 0 |
| Isopropyl alcohol | 5194 | 4710 - 5500 | 5 | 1) HSDB<br>2) EHC 103, 1990 | 0 |
| Isopropylidenediphenol:p,p'- | 4018 | 3200 - 5660 | 9 | 1) HSDB<br>2) IUCLID | 0 |
| Lithium carbonate | 525 | | 1 | IUCLID | 0 |
| Maleic anhydride | 648 | 235 - 1090 | 11 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO<br>4) IUCLID | 0 |
| Methanol | 8499 | 5628 - 13000 | 7 | 1) EHC 196, 1997<br>2) CHEMINFO | 0 |
| Methyl ethyl ketone | 2679 | 800 - 5520 | 7 | 1) HSDB<br>2) EHC 143, 1992<br>3) CESARS | 0 |
| Methyl isobutyl ketone | 3093 | 2080 - 4600 | 2 | 1) HSDB<br>2) CESARS | 0 |
| Methyl methacrylate | 8362 | 7800 - 9400 | 4 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |
| Methyl tert-butyl ether | 3518 | 2963 - 3866 | 3 | 1) EHC 206, 1998<br>2) CHEMINFO | 0 |

| Chemical | $LD_{50}$ (mg/kg) | $LD_{50}$ range | N | Reference(s) | $UF_{OR}$ |
|---|---|---|---|---|---|
| Methyl-2-pyrrolidone:N- | 4668 | 3598 - 7900 | 12 | 1) HSDB<br>2) CESARS<br>3) IUCLID | 0 |
| Methylenebis (phenylisocyanate) | >10000 | | 1 | 1) CHEMINFO | 0 |
| Naphthalene | 1974 | 1100 - 2600 | 6 | 1) HSDB<br>2) CESARS | 0 |
| Nitrate ion [3] | 1386 | 1200 - 1600 | 2 | IUCLID (Studies conducted on various salts of nitric acid: $NaNO_3$, $KNO_3$, $NH_4NO_3$.) | 0 |
| Nitric acid | 430 | | 1 | IUCLID (human LDLo) | 2 |
| Nitrilotriacetic acid [1] | | | | No information, default value ($HV_{OR}$=2.5) | 4 |
| Nonylphenol | 1511 | 580 - 2462 | 11 | 1) PSL Assessment 2000<br>2) IUCLID | 0 |
| Phenol (and its salts) | 462 | 317 - 650 | 9 | 1) HSDB<br>2) EHC 161, 1994<br>3) CESARS | 0 |
| Phosphorus [4] | 3.03 | 3.03 - 3.03 | 1 | HSDB | 0 |
| Phthalic anhydride | 1726 | 800 - 4020 | 3 | 1) HSDB<br>2) CESARS | 0 |
| Polymeric diphenylmethane diisocyanate | >10000 | | 1 | CHEMINFO | 0 |
| Propylene | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely since propylene is a gas at room temperature, medium of concern is air and more than 99% of NPRI releases are to air. | 1 |
| Sodium fluoride | 41 | 32 - 51.6 | 2 | HSDB | 0 |
| Sodium nitrite | 145 | 85 - 200 | 3 | IUCLID | 0 |
| Styrene | 2236 | 1000 - 5000 | 2 | HSDB | 0 |
| Sulphur hexafluoride | | | | Expert judgement ($HV_{OR}$=0); ingestion unlikely since gas at room temperature and medium of concern is air. | 1 |
| Sulphuric acid | 2140 | | 1 | CHEMINFO | 0 |

| Chemical | $LD_{50}$ (mg/kg) | $LD_{50}$ range | N | Reference(s) | $UF_{OR}$ |
|---|---|---|---|---|---|
| Tetrachloroethylene | 2433 | 250 - 13000 | 9 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO<br>4) IUCLID | 0 |
| Thiourea | 564 | 20 - 6200 | 6 | 1) HSDB<br>2) IUCLID | 0 |
| Toluene | 5289 | 2600 - 7530 | 11 | 1) HSDB<br>2) EHC 52, 1986<br>3) CHEMINFO | 0 |
| Toluene-2,4-diisocyanate | 5982 | 5800 - 6170 | 2 | 1) HSDB<br>2) CESARS | 0 |
| Toluenediisocyanate [5] | 4842 | 3060 - 7500 | 4 | 1) HSDB<br>2) CESARS | 0 |
| Trichloroethylene | 4398 | 2402 - 7200 | 3 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |
| Triethylamine | 460 | | 1 | 1) CESARS | 0 |
| Trimethylbenzene:1,2,4- | 3876 | 3280 - 5000 | 3 | 1) CHEMINFO<br>2) HSDB | 0 |
| Vinyl acetate | 2920 | | 1 | HSDB | 0 |
| Vinyl chloride | >4000 | | 1 | IUCLID | 0 |
| Xylene [5] | 5657 | 3523 - 8700 | 8 | 1) HSDB<br>2) EHC 190, 1997<br>3) CESARS<br>4) CHEMINFO | 0 |

[1] and its salts

[2] mixed isomers and their salts

[3] in solution at pH ≥ 6.0

[4] yellow or white

[5] mixed isomers

**Rat 4-hour Inhalation $LC_{50}$**

| Chemical | $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference(s) | $UF_{INH}$ |
|---|---|---|---|---|---|
| Acetaldehyde | 19.41 | 15.7 - 24 | 2 | 1) CHEMINFO<br>2) EHC 167, 1995/ IUCLID | 0 |
| Acrolein | 0.02 | 0.018 - 0.021 | 2 | 1) CESARS<br>2) EHC 127, 1991 | 0 |
| Acrylamide | 1.4 | | | Green Seal | 2 |
| Acrylic acid [1] | 3.71 | 3.60 - 3.83 | 2 | CHEMINFO | 0 |
| Acrylonitrile | 1.10 | 0.92 - 1.30 | 3 | 1) CESARS<br>2) CHEMINFO<br>3) IUCLID | 0 |
| Ammonia | 1.39 | | 1 | IUCLID | 0 |
| Anthracene | | | | Expert judgement ($HV_{INH}$=0); inhalation unlikely as anthracene is not likely to form vapour. | 1 |
| Benzene | 43.77 | | 1 | CHEMINFO/ IUCLID | 0 |
| Benzoyl peroxide | | | | Expert judgement ($HV_{INH}$=0); not likely to present inhalation risk as media of concern are soil and water. | 1 |
| Biphenyl | 30.5 | | | Green Seal | 2 |
| Bis(2-ethylhexyl) adipate | | | | Expert judgement ($HV_{INH}$=0); inhalation unlikely pathway as Henry's Law predicts low volatility and media of concern are soil, sediment, and water. | 1 |
| Bis(2-ethylhexyl) phthalate | > 10.62 | | 1 | IUCLID | 0 |
| Bromine | 21.7 | | | Green Seal | 2 |
| Butadiene:1,3- | 285 | | 1 | HSDB/ IUCLID | 0 |
| Butoxyethanol:2- | 2.26 | 2.18 - 2.35 | 2 | CHEMINFO | 0 |
| Butyl acrylate | 14.31 | | 1 | CHEMINFO | 0 |
| Butyl alcohol:i- | 25.30 | 24.3 - 26.4 | 2 | 1) HSDB<br>2) CESARS | 0 |
| Butyl alcohol:n- | 24.25 | | 1 | HSDB | 0 |
| Butyl alcohol:sec- | 24.25 | | | Read-across from n-butyl alcohol | 2 |
| Butyl alcohol:tert- | > 30.32 | | 1 | IUCLID | 0 |
| Butyl benzyl phthalate | > 6.7 | | 1 | IUCLID | 0 |

| Chemical | $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference(s) | $UF_{INH}$ |
|---|---|---|---|---|---|
| Calcium fluoride | 35.4 | | | Green Seal | 2 |
| Carbon disulphide | 12.5 | | 1 | HSDB | 2 |
| Carbon tetrachloride | 50.33 | | 1 | IUCLID | 0 |
| Chlorine | 0.27 | 0.22 - 0.33 | 2 | 1) HSDB<br>2) IUCLID | 2 |
| Chlorine dioxide | 2.4 | | | Green Seal | 2 |
| Chlorobenzene | 11.65 | 8.58 - 13.65 | 3 | 1) EHC 128, 1991<br>2) CHEMINFO | 0 |
| Chloroform | 47.70 | | 1 | HSDB | 0 |
| Chloromethane | 5.3 | | 1 | HSDB | 0 |
| Cresol [2] | 12.1 | | | Green Seal | 2 |
| Cumene | 39.2 | | 1 | CESARS | 0 |
| Cumene hydroperoxide | 1.37 | | 1 | IUCLID | 0 |
| Cyanide ion | 0.02 | | | HCN used as a surrogate to estimate $CN^-$ inhalation toxicity as $CN^-$ likely forms HCN when emitted to air. | 2 |
| Cyclohexane | 13.9 | | 1 | IUCLID | 0 |
| Decabromodiphenyl oxide | 12.05 | | 1 | IUCLID | 2 |
| Dibutyl phthalate | > 15.68 | | 1 | IUCLID | 0 |
| Dichlorobenzene:p- | 17.3 | | | Green Seal | 2 |
| Dichloroethane:1,2- | 8.4 | | 1 | CESARS | 0 |
| Dichloromethane | > 2 | | | 1) HSDB<br>2) CESARS | 0 |
| Dicyclopentadiene | 3.82 | 2.70 - 5.41 | 2 | 1) IUCLID | 0 |
| Diethanolamine [1] | | | | Expert judgement ($HV_{INH}$=0); inhalation pathway unlikely as Henry's Law predicts low volatility and media of concern are soil and water. | 1 |
| Dimethylformamide:n,n- | > 5.9 | | 1 | IUCLID | 0 |
| Dioxane:1,4- | 48.60 | 46 - 51.4 | 2 | 1) CESARS<br>2) CHEMINFO | 0 |
| Di-t-butyl-4-methylphenol:2,6- | | | | Expert judgement ($HV_{INH}$=0); inhalation unlikely pathway as media of concern are soil and water and only 1% of NPRI releases are to air. | 1 |

| Chemical | $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference(s) | $UF_{INH}$ |
|---|---|---|---|---|---|
| Ethyl acrylate | 5.74 | 3.6 - 8.93 | 5 | 1) HSDB<br>2) CHEMINFO<br>3) EHC 191, 1997 | 0 |
| Ethylbenzene | 17.2 | | 1 | EHC 186, 1996 | 0 |
| Ethylene | > 12.52 | | 1 | IUCLID | 0 |
| Ethylene glycol | | | | Expert judgement ($HV_{INH}$ = 0); inhalation pathway unlikely as Henry's Law predicts low volatility and media of concern are soil and water. | 1 |
| Ethylene oxide | 2.63 | | 1 | HSDB/ PSL Assessment 2001 | 0 |
| Fluorine | 0.06 | | 1 | HSDB | 3 |
| Formaldehyde | 0.44 | 0.31 - 0.59 | 3 | 1) HSDB<br>2) CESARS | 0 |
| Formic acid | 5.28 | 3.76 - 7.4 | 2 | 1) CHEMINFO<br>2) IUCLID | 0 |
| HCFC-141b | 295 | | 1 | HSDB | 0 |
| HCFC-142b | 1644.17 | | | IUCLID | 0 |
| HCFC-22 | 775 | | 1 | EHC 126, 1991/ IUCLID | 0 |
| Hexane:n- | 209.73 | 169.18 - 260 | 2 | CESARS | 0 |
| Hydrochloric acid | 0.93 | 0.56 - 1.18 | 6 | 1) IUCLID<br>2) CHEMINFO | 2 |
| Hydrogen cyanide | 0.02 | 0.02 - 0.04 | 4 | 1) HSDB/IUCLID<br>2) IUCLID | 2 |
| Hydrogen fluoride | 0.32 | 0.21 - 0.48 | 7 | 1) HSDB<br>2) CHEMINFO<br>3) IUCLID | 2 |
| Hydrogen sulphide | 0.66 | 0.63 - 0.70 | 2 | 1) CESARS<br>2) IUCLID | 0 |
| Hydroquinone [1] | | | | Expert judgement ($HV_{INH}$ = 0); inhalation pathway unlikely as Henry's Law predicts low volatility, medium of concern is water and 100% of NPRI releases are to water. | 1 |
| Isoprene | 180 | | 1 | HSDB/ IUCLID | 0 |
| Isopropyl alcohol | 55.07 | 41.8 - 72.6 | 2 | 1) EHC 103, 1990<br>2) CHEMINFO | 0 |

| Chemical | $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference(s) | $UF_{INH}$ |
|---|---|---|---|---|---|
| Isopropylidenediphenol:p,p'- | | | | Expert judgement ($HV_{INH}$ = 0); inhalation pathway unlikely as Henry's Law predicts low volatility, medium of concern is soil and 93% of NPRI releases are to land. | 1 |
| Lithium carbonate | > 2.17 | | 1 | IUCLID | 0 |
| Maleic anhydride | 5.4 | | | Green Seal | 2 |
| Methanol | 83.87 | | 1 | CHEMINFO | 0 |
| Methyl ethyl ketone | 11.72 | 3.98 - 34.5 | 2 | 1) HSDB<br>2) CESARS | 0 |
| Methyl isobutyl ketone | 23.13 | 16.35 - 32.71 | 2 | CESARS | 0 |
| Methyl methacrylate | 29.04 | | 1 | IUCLID | 0 |
| Methyl tert-butyl ether | 85 | | 1 | HSDB | 0 |
| Methyl-2-pyrrolidone:N- | 5.18 | 3.1 - 8.8 | 3 | IUCLID | 0 |
| Methylenebis (phenylisocyanate) | 0.41 | 0.37 - 0.49 | 3 | 1) HSDB<br>2) CHEMINFO | 0 |
| Naphthalene | 1.05 | | 1 | IUCLID | 2 |
| Nitrate ion [3] | 0.17 | | 1 | $HNO_3$ used as surrogate as $NO_3^-$ likely forms $HNO_3$ when emitted to air. | 2 |
| Nitric acid | 0.17 | | 1 | HSDB | 0 |
| Nitrilotriacetic acid [1] | | | | Expert judgement ($HV_{INH}$ = 0); not relevant route of exposure. | 1 |
| Nonylphenol | | | | Expert judgement ($HV_{INH}$ = 0); inhalation pathway unlikely as fugacity modelling indicates media of concern are water and soil. Further, air is not considered a compartment of concern in PSL environmental risk assessment. | 1 |
| Phenol [1] | > 1.8 | | 1 | IUCLID | 2 |
| Phosphorus [4] | 1.08 | | 1 | IUCLID | 2 |
| Phthalic anhydride | | | | Expert judgement ($HV_{INH}$ = 0); inhalation pathway unlikely as Henry's Law predicts low volatility, media of concern are soil and water and 99% of NPRI releases are to water. | 1 |
| Polymeric diphenylmethane diisocyanate | 0.49 | | 1 | CHEMINFO | 0 |
| Propylene | > 86 | | 1 | CHEMINFO | 0 |

| Chemical | $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference(s) | $UF_{INH}$ |
|---|---|---|---|---|---|
| Sodium fluoride | | | | Expert judgement ($HV_{INH}$ = 0); inhalation pathway unlikely as media of concern are soil and water and 100% of NPRI releases are to land. | 1 |
| Sodium nitrite | 5.5 | | 1 | IUCLID | 0 |
| Styrene | 16.83 | 11.8 - 24 | 2 | HSDB | 0 |
| Sulphur hexafluoride | 5.97 | | 1 | CHEMINFO | 0 |
| Sulphuric acid | 0.26 | | 1 | CHEMINFO | 0 |
| Tetrachloroethylene | 27.13 | | 1 | IUCLID | 0 |
| Thiourea | > 0.9 | | 1 | IUCLID | 0 |
| Toluene | 30.4 | 28.1 - 33.2 | 3 | 1) HSDB<br>2) CHEMINFO<br>3) IUCLID | 0 |
| Toluene-2,4-diisocyanate | 0.1 | | 1 | HSDB | 0 |
| Toluenediisocyanate [5] | 0.23 | 0.10 - 0.36 | 3 | HSDB | 0 |
| Trichloroethylene | 57.09 | 43.0 - 67.2 | 3 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |
| Triethylamine | 4.14 | | 1 | HSDB | 0 |
| Trimethylbenzene:1,2,4- | 18 | | 1 | CHEMINFO | 0 |
| Vinyl acetate | 12.89 | 11.4 - 14.4 | 3 | 1) HSDB<br>2) CHEMINFO | 0 |
| Vinyl chloride | 86.14 | | 1 | CHEMINFO | 0 |
| Xylene [5] | 55.62 | 28 - 104 | 6 | 1) HSDB<br>2) CESARS<br>3) CHEMINFO | 0 |

[1] and its salts

[2] mixed isomers and their salts

[3] in solution at pH ≥ 6.0

[4] yellow or white

[5] mixed isomers

## Carcinogenicity Rating

| Chemical | Carcinogenicity Rating | Reference(s) | $UF_{CAR}$ |
|---|---|---|---|
| Acetaldehyde | 2B | IARC. VOL.: 71 (1999) (p. 319) | 0 |
| Acrolein | 3 | IARC. VOL.: 63 (1995) (p. 337) | 0 |
| Acrylamide | 2A | IARC. VOL.: 60 (1994) (p. 389) | 0 |
| Acrylic acid [1] | 3 | IARC. VOL.: 71 (1999) (p. 1223) | 0 |
| Acrylonitrile | 2B | IARC. VOL.: 71 (1999) (p. 43) | 0 |
| Ammonia | 3 | EHC 54, 1986. | 2 |
| Anthracene | 3 | IARC. Suppl. 7 (1987) (p. 57: Group 3) | 0 |
| Benzene | 1 | IARC. Supplement 7: (1987) (p. 120) | 0 |
| Benzoyl peroxide | 3 | IARC. VOL.: 71 (1999) (p. 345) | 0 |
| Biphenyl | 2A | IARC. Supplement 7: (1987) (p. 322) | 0 |
| Bis(2-ethylhexyl) adipate | 3 | IARC. Vol.: 77 (2000) (p. 149) | 0 |
| Bis(2-ethylhexyl) phthalate | 3 | IARC. VOL.: 77 (2000) (p. 41) | 0 |
| Bromine | 3 | IUCLID dataset. Section 5.7 concludes residues of up to 500 ppm total bromine in diets fumigated with methyl bromide are not carcinogenic in F344 rats and there was no evidence of bromine having carcinogenic properties. | 2 |
| Butadiene:1,3- | 2A | IARC VOL.: 71 (1999) (p. 109) | 0 |
| Butoxyethanol:2- | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Butyl acrylate | 3 | IARC. VOL.: 71 (1999) (p. 359) | 0 |
| Butyl alcohol:i- | D | read-across assessment for 1-butanol (71-36-3) | 2 |
| Butyl alcohol:n- | D | IRIS. 03/01/1991 | 0 |
| Butyl alcohol:sec- | D | read-across assessment for 1-butanol (71-36-3) | 2 |
| Butyl alcohol:tert- | D | read-across assessment for 1-butanol (71-36-3) | 2 |
| Butyl benzyl phthalate | 3 | IARC. VOL.: 73 (1999) (p. 115) | 0 |
| Calcium fluoride | 3 | PSL assessment. No consistent evidence. | 2 |
| Carbon disulphide | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Carbon tetrachloride | 2B | IARC. Vol.: 71 (1999) (p. 401). IRIS. 06/01/1991 | 0 |
| Chlorine | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 01/01/1993. Carcinogenicity assessment unavailable. | 4 |
| Chlorine dioxide | D | IRIS. 10/12/2000 | 0 |
| Chlorobenzene | D | IRIS. 03/01/1991 | 0 |

| Chemical | Carcinogenicity Rating | Reference(s) | $UF_{CAR}$ |
|---|---|---|---|
| Chloroform | 2B | IARC. VOL.: 73 (1999) (p. 131). IRIS. 10/19/01 | 0 |
| Chloromethane | 3 | IARC. VOL.: 71 (1999) (p. 737). | 0 |
| Cresol [2] | C | IRIS. 08/01/1993 | 0 |
| Cumene | D | IRIS. 08/01/1997 | 0 |
| Cumene hydroperoxide | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Cyanide ion | D | IRIS. 03/01/1991 | 0 |
| Cyclohexane | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 09/11/2003. Carcinogenicity assessment unavailable. | 4 |
| Decabromodiphenyl oxide | 3 | IARC. VOL.: 71 (1999) (p. 1365). | 0 |
| Dibutyl phthalate | D | IRIS. 02/01/1993 | 0 |
| Dichlorobenzene:p- | 2B | IARC. VOL.: 73 (1999) (p. 223) | 0 |
| Dichloroethane:1,2- | 2B | IARC. VOL.: 71 (1999) (p. 501) | 0 |
| Dichloromethane | 2B | IARC. VOL.: 71 (1999) (p. 251) | 0 |
| Dicyclopentadiene | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Diethanolamine [1] | 3 | IARC. VOL.: 77 (2000) (p. 349) | 0 |
| Dimethylformamide:n,n- | 3 | IARC. VOL.: 71 (1999) (p. 545) | 0 |
| Dioxane:1,4- | 2B | IARC. VOL.: 71 (1999) (p. 589) | 0 |
| Di-t-butyl-4-methylphenol:2,6- | 3 | IARC. Suppl. 7 (1987) (p. 59) | 0 |
| Ethyl acrylate | 2B | IARC. VOL.: 71 (1999) (p. 1447) | 0 |
| Ethylbenzene | 2B | IARC. Vol.: 77 (2000) (p. 227). | 0 |
| Ethylene | 3 | IARC. VOL.: 60 (1994) (p. 45) | 0 |
| Ethylene glycol | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Ethylene oxide | 1 | IARC. VOL.: 60 (1994) (p. 73) | 0 |
| Fluorine | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Formaldehyde | 2A | IARC. Vol.: 62 (1995) (p. 217) | 0 |
| Formic acid | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 10/01/1991. Carcinogenicity assessment unavailable. | 4 |
| HCFC-141b | 3 | Read-across IARC assessment for HCFC-22. | 2 |

| Chemical | Carcinogenicity Rating | Reference(s) | $UF_{CAR}$ |
|---|---|---|---|
| HCFC-142b | 3 | Read-across IARC assessment for HCFC-22. | 2 |
| HCFC-22 | 3 | IARC. VOL.: 71 (1999) (p. 1339) | 0 |
| Hexane:n- | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 09/01/1991. Carcinogenicity assessment unavailable. | 4 |
| Hydrochloric acid | 3 | IARC. VOL.: 54 (1992) (p. 189) | 0 |
| Hydrogen cyanide | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Hydrogen fluoride | 3 | PSL assessment. No consistent evidence | 2 |
| Hydrogen sulphide | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 07/28/2003. Carcinogenicity assessment unavailable. | 4 |
| Hydroquinone [1] | 3 | IARC. VOL.: 71 (1999) (p. 691) | 0 |
| Isoprene | 2B | IARC. VOL.: 71 (1999) (p. 1015) | 0 |
| Isopropyl alcohol | 3 | IARC. VOL.: 71 (1999) (p. 1027) | 0 |
| Isopropylidenediphenol:p,p'- | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Lithium carbonate | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Maleic anhydride | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Methanol | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Methyl ethyl ketone | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 09/26/2003. Carcinogenicity assessment not available. | 4 |
| Methyl isobutyl ketone | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 04/25/2003. Carcinogenicity assessment not available. | 4 |
| Methyl methacrylate | 3 | IARC. VOL.: 60 (1994) (p. 445) | 0 |
| Methyl tert-butyl ether | 3 | IARC. VOL.: 73 (1999) (p. 339) | 0 |
| Methyl-2-pyrrolidone:N- | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Methylenebis (phenylisocyanate) | 3 | IARC. VOL.: 71 (1999) (p. 1049) | 0 |
| Naphthalene | C | IRIS. 09/17/1998 | 0 |
| Nitrate ion [3] | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Nitric acid | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Nitrilotriacetic acid [1] | 2B | IARC. VOL.: 73 (1999) (p. 385) | 0 |
| Nonylphenol | C | PSL assessment does not rule on carcinogenicity. Nonylphenol negative in bacterial tests, but induced DNA damage in human sperm, lymphocytes and MCF-7 breast cancer cells exposed in vitro. | 2 |
| Phenol [1] | 3 | IARC. VOL.: 71 (1999) (p. 749) | 0 |
| Phosphorus [4] | - | No information, default value ( $HV_{CAR}$ = 1.5) | 4 |

| Chemical | Carcinogenicity Rating | Reference(s) | $UF_{CAR}$ |
|---|---|---|---|
| Phthalic anhydride | - | No information, default value ($HV_{CAR}$ = 1.5). IRIS. 05/01/1992. Carcinogenicity assessment not available. | 4 |
| Polymeric diphenylmethane diisocyanate | D | IRIS. 02/07/1998 | 0 |
| Propylene | 3 | IARC. VOL.: 60 (1994) (p. 161) | 0 |
| Sodium fluoride | 3 | IARC. Supplement 7: (1987) (p. 208) | 0 |
| Sodium nitrite | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Styrene | 2B | IARC. VOL.: 60 (1994) (p. 233) | 0 |
| Sulphur hexafluoride | 3 | PSL assessment. No consistent evidence. | 2 |
| Sulphuric acid | 1 | IARC. VOL.: 54 (1992) (p. 41) | 0 |
| Tetrachloroethylene | 2A | IARC. VOL.: 63 (1995) (p. 159) | 0 |
| Thiourea | 3 | IARC. VOL.: 79 (2001) (p. 703). | 0 |
| Toluene | 3 | IARC. VOL.: 71 (1999) (p. 829) | 0 |
| Toluene-2,4-diisocyanate | 2B | IARC. VOL.: 71 (1999) (p. 865) | 0 |
| Toluenediisocyanate [5] | 2B | IARC. VOL.: 71 (1999) (p. 865) | 0 |
| Trichloroethylene | 2A | IARC. Vol.: 63 (1995) (p. 75) | 0 |
| Triethylamine | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Trimethylbenzene:1,2,4- | - | No information, default value ($HV_{CAR}$ = 1.5) | 4 |
| Vinyl acetate | 2B | IARC. VOL.: 63 (1995) (p. 443) | 0 |
| Vinyl chloride | 1 | IARC. Supplement 7: (1987) (p. 373) | 0 |
| Xylene [5] | 3 | IARC. VOL.: 71 (1999) (p. 1189) | 0 |

[1] and its salts

[2] mixed isomers and their salts

[3] in solution at pH ≥ 6.0

[4] yellow or white

[5] mixed isomers

**Reference Dose/Reference Concentration**

| Chemical | Study | NOAEL/C [1] | LOAEL/C | Uncertainty Factor | RfD/RfC | $UF_{NCAR}$ | Reference |
|---|---|---|---|---|---|---|---|
| Acetaldehyde | 4-week rat | 8.775 | | 1000 | 0.009 | 0 | RfC. IRIS. 10/01/1991. |
| Acrolein | 13-week rat | | 0.023 | 1000 | 0.000 | 0 | RfC. IRIS. 06/03/2003. |
| Acrylamide | 90-day rat | 0.2 | | 1000 | 0.000 | 0 | RfD. IRIS. 03/01/1991. |
| Acrylic acid [2] | 13-week mouse | | 0.325 | 300 | 0.001 | 0 | RfC. IRIS.05/01/1995. |
| Acrylonitrile | 2-year rat | | 1.940 | 1000 | 0.002 | 0 | RfC. IRIS.12/01/1991. |
| Ammonia | 12.2-year human | 2.3 | | 30 | 0.077 | 0 | RfC. IRIS 05/01/1991. |
| Anthracene | 90-day mouse | 1000 | | 3000 | 0.333 | 0 | RfD. IRIS. 07/01/1993. |
| Benzene | 6.3-year human occupational | 8.2 | | 300 | 0.027 | 0 | RfC. IRIS. 04/17/2003. |
| Benzoyl peroxide | exposure limit | 5 | | 1 | 5.000 | 2 | RfC. CHEMINFO/ CHRIS (Exposure limit = 5 $mg/m^3$) |
| Biphenyl | chronic rat | 50 | | 1000 | 0.050 | 0 | RfD. IRIS. 08/01/1989. |
| Bis(2-ethylhexyl) adipate | developmental/ 1-generation rat | 170 | | 300 | 0.567 | 0 | RfD. IRIS. 07/01/1992. |
| Bis(2-ethylhexyl) phthalate | 1-year guinea pig | | 19.000 | 1000 | 0.019 | 0 | RfD. IRIS. 05/01/1991. |
| Bromine | exposure limit | 0.654 | | 1 | 0.654 | 2 | RfC. CHEMINFO/ CHRIS (Exposure limit = 0.1 ppm) |
| Butadiene:1,3- | 2-year mouse | | 1.950 | 1000 | 0.002 | 0 | RfC. IRIS. 11/05/2002. |
| Butoxyethanol:2- | 14-week rat | | 380.000 | 30 | 12.667 | 0 | RfC. IRIS. 12/30/1999. |
| Butyl acrylate | 2-year rat | | 14.000 | 300 | 0.047 | 2 | RfC. HSDB. |
| Butyl alcohol:i- | 13-week rat | 316 | | 1000 | 0.316 | 0 | RfD. IRIS. 04/01/1999. |
| Butyl alcohol:n- | 13-week rat | 125 | | 1000 | 0.125 | 0 | RfD. IRIS. 09/01/1990. |
| Butyl alcohol:sec- | multi-generation reproductive/ development rat | 657 | | 300 | 2.190 | 0 | RfD. IRIS (see methyl ethyl ketone assessment). 9/26/2003. |
| Butyl alcohol:tert- | 2-year rat/mouse | | 180.000 | 1000 | 0.180 | 2 | RfD. CHEMINFO. |
| Butyl benzyl phthalate | 6-month rat | 159 | | 1000 | 0.159 | 0 | RfD. IRIS. 02/01/1993. |
| Calcium fluoride | occupational studies (+20year) | 0.2 | | 100 | 0.002 | 2 | RfD. PSL Assessment for Inorganic Fluorides. 1993. |
| Carbon disulphide | 12.1-year occupational | | 19.700 | 30 | 0.657 | 0 | RfC. IRIS. 08/01/1995. |

| Chemical | Study | NOAEL/C [1] | LOAEL/C | Uncertainty Factor | RfD/RfC | $UF_{NCAR}$ | Reference |
|---|---|---|---|---|---|---|---|
| Carbon tetrachloride | 12-week rat | 0.71 | | 1000 | 0.001 | 0 | RfD. IRIS. 06/01/1991. |
| Chlorine | 2-year rat | 14.4 | | 100 | 0.144 | 0 | RfD. IRIS. 06/01/1994. |
| Chlorine dioxide | 2-month rat | | 0.645 | 3000 | 0.000 | 0 | RfC. IRIS 10/12/2000. |
| Chlorobenzene | 13-week dog | 27.25 | | 1000 | 0.027 | 0 | RfD. IRIS. 07/01/1993. |
| Chloroform | 7.5-year dog | 1 | | 100 | 0.010 | 0 | RfD. IRIS. 10/19/2001. |
| Chloromethane | 11-day continuous mouse | 94.6 | | 1000 | 0.095 | 0 | RfC. IRIS. 07/17/2001. |
| Cresol [3] | 90-day neurotoxicity rat | 50 | | 1000 | 0.050 | 0 | RfD. IRIS (o-, m-cresol). 09/10/1990. |
| Cumene | 13-week rat | 435 | | 1000 | 0.435 | 0 | RfC. IRIS. 08/01/1997. |
| Cumene hydroperoxide | 90-day rat | 6 | 22.143 | 300 | 0.018 | 2 | RfC. HSDB. |
| Cyanide ion | 2-year/ subchronic rat | 10.8 | | 500 | 0.022 | 0 | RfD. IRIS. 02/01/1993. |
| Cyclohexane | 2-generation reproductive rat | 1822 | | 300 | 6.073 | 0 | RfC. IRIS. 09/11/2003. |
| Decabromodiphenyl oxide | 2-year rat | 1 | | 100 | 0.010 | 0 | RfD. IRIS. 02/01/1995. |
| Dibutyl phthalate | 1-year rat | 125 | | 1000 | 0.125 | 0 | RfD. IRIS. 08/01/1990. |
| Dichlorobenzene:p- | 2-generation reproductive rat | 75 | | 100 | 0.750 | 0 | RfC. IRIS. 11/01/1996. |
| Dichloroethane:1,2- | Maximum Residue Limit | | | | 2.428 | 0 | RfC. ATSDR (MRL = 0.6 ppm). Sept. 2001. |
| Dichloromethane | 2-year rat | 5.85 | | 100 | 0.059 | 0 | RfD. IRIS. 03/01/1988. |
| Dicyclopentadiene | exposure limit | 27 | | 1 | 27.036 | 2 | RfC. CHEMINFO/CHRIS.(Exposure limit = 5 ppm) |
| Diethanolamine [2] | 90-day rat/mouse | | 15.000 | 1000 | 0.015 | 2 | RfD. NTP technical report on toxicity studies of diethanolamine (CAS No. 111-42-2) administered topically and in drinking water to F344/N rats and $B6C3F_1$ mice. 1992. National Toxicology Program, Toxicity Report Series No. 20, NIH publication No. 92-3343. U.S. Department of Health and Human Services. |
| Dimethylformamide:n,n- | 5 (1-15) year occupational | | 7.900 | 300 | 0.026 | 0 | RfC. IRIS. 10/01/1990. |
| Dioxane:1,4- | 2-year rat | 9.6 | | 300 | 0.032 | 2 | RfD. CHEMINFO. |

| Chemical | Study | NOAEL/C [1] | LOAEL/C | Uncertainty Factor | RfD/RfC | $UF_{NCAR}$ | Reference |
|---|---|---|---|---|---|---|---|
| Di-t-butyl-4-methylphenol:2,6- | 2-geneneration rat | | 25.000 | 1000 | 0.025 | 2 | RfD. HSDB. |
| Ethyl acrylate | 2-year rat | 102 | | 100 | 1.024 | 2 | RfC. CHEMINFO. |
| Ethylbenzene | developmental rabbit/rat | 434 | | 300 | 1.447 | 0 | RfC. IRIS. 03/01/1991. |
| Ethylene | 2-year rat | 615 | | 300 | 2.049 | 2 | RfC. HSDB. |
| Ethylene glycol | 2-year rat | 200 | | 100 | 2.000 | 0 | RfD. IRIS. 09/01/1989. |
| Ethylene oxide | 2-year rat | | 2.200 | 1000 | 0.002 | 2 | RfC. PSL Assessment. Sept. 2001. |
| Fluorine | occupational (children) | 0.06 | | 1 | 0.060 | 0 | RfD. IRIS. 06/01/1989. |
| Formaldehyde | 2-year rat | 15 | | 100 | 0.150 | 0 | RfD. IRIS. 09/01/1990. |
| Formic acid | 13-week rat/ mouse | 10.8 | | 1000 | 0.011 | 2 | RfC. NTP technical report on toxicity studies of formic acid (CAS no: 64-18-6) administered by inhalation to F344/N rats and $B6C3F_1$ mice. 1992. National Toxicology Program, Technical Report Series No. 19. U.S. Department of Health and Human Services. |
| HCFC-141b | 2-year rat | 1,281 | | 100 | 12.812 | 2 | RfC. HSDB. |
| HCFC-142b | 2-year rat | 14710 | | 300 | 49.033 | 0 | RfC. IRIS. 07/01/1995. |
| HCFC-22 | 2-year/ developmental rat | 5260 | | 100 | 52.600 | 0 | RfC. IRIS. 11/01/1993. |
| Hexane:n- | 6.2 (1-12) year occupational | | 73.000 | 300 | 0.243 | 0 | RfC. IRIS. 07/01/1993. |
| Hydrochloric acid | chronic rat | | 6.100 | 300 | 0.020 | 0 | RfC. IRIS. 07/01/1995. |
| Hydrogen cyanide | 5-10 year occupational | | 7.070 | 1000 | 0.007 | 0 | RfC. IRIS. 09/01/1994. |
| Hydrogen fluoride | Maximum Residue Limit | | | | 0.016 | 0 | RfC. ATSDR (MRL = 0.02 ppm). Sept. 2003. |
| Hydrogen sulphide | 10-week rat | 0.64 | | 300 | 0.002 | 0 | RfC. IRIS. 07/28/2003. |

| Chemical | Study | NOAEL/C [1] | LOAEL/C | Uncertainty Factor | RfD/RfC | $UF_{NCAR}$ | Reference |
|---|---|---|---|---|---|---|---|
| Hydroquinone [2] | 2-year rat/ mouse | | 25.000 | 1000 | 0.025 | 2 | RfD. NTP Technical report on the toxicology and carcinogenesis studies of hydroquinone (CAS No. 123-31-9) in F344/N rats and B6C3F1 mice (gavage studies). 1989. National Toxicology Program, Technical Report Series No. 336, NIH Publication No. 90-2812, U.S Department of Health and Human Services. |
| Isoprene | 2-year mouse | | 1.950 | 1000 | 0.002 | 2 | RfC. IRIS (1,3-butadiene). 11/05/2002. |
| Isopropyl alcohol | 2-year rat/ 16-month mouse | 219 | | 100 | 2.195 | 2 | RfC. CHEMINFO. |
| Isopropylidenediphenol:p,p'- | 2-year rat | | 50.000 | 1000 | 0.050 | 0 | RfD. IRIS. 07/01/1993. |
| Lithium carbonate | | | | | | 4 | No information, default value ($HV_{NCAR}$=2.5) |
| Maleic anhydride | 2-year/multi-generation rat | 10 | 20.000 | 100 | 0.100 | 0 | RfD. IRIS. 07/01/1993. |
| Methanol | 90-day rat | 500 | | 1000 | 0.500 | 0 | RfD. IRIS. 07/01/1993. |
| Methyl ethyl ketone | Developmental rat/mouse | 1517 | | 300 | 5.057 | 0 | RfC. IRIS. 09/26/2003. |
| Methyl isobutyl ketone | Developmental rat/mouse | 1026 | | 300 | 3.420 | 0 | RfC. IRIS. 04/25/2003. |
| Methyl methacrylate | 2-year rat | 7.2 | | 10 | 0.720 | 0 | RfC. IRIS. 03/02/1998. |
| Methyl tert-butyl ether | 2-year rat | 259 | | 100 | 2.590 | 0 | RfC. IRIS. 09/01/1993. |
| Methyl-2-pyrrolidone:N- | 28-day rat | 300 | | 1000 | 0.300 | 2 | RfD. HSDB. |
| Methylenebis (phenylisocyanate) | 2-year rat | 0.06 | | 100 | 0.001 | 0 | RfC. IRIS. 02/07/1998. |
| Naphthalene | 2-year mouse | | 9.300 | 3000 | 0.003 | 0 | RfC. IRIS. 02/17/1998. |
| Nitrate ion [4] | epidemiological surveys | 1.6 | | 1 | 1.600 | 0 | RfD. IRIS. 10/01/1991. |
| Nitric acid | exposure limit | 5 | | 1 | 5.154 | 2 | RfC. CHEMINFO. (Exposure limit = 2 ppm) |
| Nitrilotriacetic acid [2] | 18-month rat | | 375.000 | 1000 | 0.375 | 2 | RfD. HSDB. |
| Nonylphenol | 3-generation reproductive rat | 12 | | 100 | 0.120 | 2 | RfD. PSL Assessment Report for nonylphenol and its ethoxylates. December 2000. |
| Phenol [2] | developmental rat | 93 | | 300 | 0.310 | 0 | RfD. IRIS. 09/30/2002. |

| Chemical | Study | NOAEL/C [1] | LOAEL/C | Uncertainty Factor | RfD/RfC | $UF_{NCAR}$ | Reference |
|---|---|---|---|---|---|---|---|
| Phosphorus [5] | 1-generation reproductive rat | 0.015 | | 1000 | 0.000 | 0 | RfD. IRIS. 02/01/1993. |
| Phthalic anhydride | 2-year mouse | | 1562.000 | 1000 | 1.562 | 0 | RfD. IRIS. 09/07/1988. |
| Polymeric diphenylmethane diisocyanate | 2-year rat | 0.06 | | 100 | 0.001 | 0 | RfC. IRIS. 02/07/1998. |
| Propylene | 2-year rat/ mouse | | 1536.678 | 1000 | 1.537 | 2 | RfC. NTP Technical Report on the Toxicology and Carcinogenesis Studies of Propylene (CAS No. 115-07-1) in F344/N rats and $B6C3F_1$ mice. 1985. National Toxicology Program, Technical Report Series No. 272. U.S. Department of Health and Human Services. |
| Sodium fluoride | occupational studies (+20yr) | 0.2 | > 0.2 | 100 | 0.002 | 2 | RfD. PSL Assessment for Inorganic Fluorides. 1993. |
| Sodium nitrite | 2-year rat/ mouse | 70 | | 100 | 0.700 | 2 | RfD. NTP Technical Report on the Toxicology and Carcinogenesis Studies of Sodium Nitrite (CAS No. 7632-00-0) in F344/N rats and B6C3F1 mice. 2001. National Toxicology Program, Technical Report Series No. 495, NIH Publication No. 01-3954. U.S. Department of Health and Human Services. |
| Styrene | 8.6 (+/- 4.5) year occupational | 34 | | 30 | 1.133 | 0 | RfC. IRIS. 07/01/1993. |
| Sulphur hexafluoride | exposure limit | 5974 | | 1 | 5973.579 | 2 | RfC. CHEMINFO. (Exposure limit = 1000 ppm) |
| Sulphuric acid | exposure limit | 1 | | 1 | 1.000 | 2 | RfC. CHEMINFO. (Exposure limit = 1 $mg/m^3$) |
| Tetrachloroethylene | 6-week rat | 14 | | 1000 | 0.014 | 0 | RfD. IRIS. 03/01/1988. |
| Thiourea | | | | | | 4 | No information, default value ($HV_{NCAR}$=2.5) |
| Toluene | 5.7 (+/- 3.2) occupational study/ 2-year rat | | 119.000 | 300 | 0.397 | 0 | RfC. IRIS. 08/01/1992. |
| Toluene-2,4-diisocyanate | prospective occupational study | 0.002 | | 30 | 0.000 | 0 | RfC. IRIS. 09/01/1995. |
| Toluenediisocyanate [6] | prospective occupational study | 0.002 | | 30 | 0.000 | 0 | RfC. IRIS. 09/01/1995. |

| Chemical | Study | NOAEL/C [1] | LOAEL/C | Uncertainty Factor | RfD/RfC | $UF_{NCAR}$ | Reference |
|---|---|---|---|---|---|---|---|
| Trichloroethylene | Maximum Residue Limit | | | | 0.537 | 0 | RfC. ATSDR (MRL = 0.1 ppm). Sept. 1997. |
| Triethylamine | 28-week/ 10-day rat | 19.5 | | 3000 | 0.007 | 0 | RfC. IRIS. 04/01/1991. |
| Trimethylbenzene:1,2,4- | 4-week rat | | 500.000 | 1000 | 0.500 | 2 | RfD. HSDB. |
| Vinyl acetate | 2-year rat/mouse | 5 | | 30 | 0.167 | 0 | RfC. IRIS. 10/01/1990. |
| Vinyl chloride | 149-week rat | 2.5 | | 30 | 0.083 | 0 | RfC. IRIS. 08/07/2000. |
| Xylene [6] | 90-day rat | 39 | | 300 | 0.130 | 0 | RfC. IRIS. 02/21/2003. |

[1] NOAEC units ($mg/m^3$); NOAEL units (mg/kg/day)

[2] and its salts

[3] mixed isomers and their salts

[4] in solution at pH ≥ 6.0

[5] yellow or white

[6] mixed isomers

**Fathead Minnow 96-hour $LC_{50}$**

| Chemical | 96-hour $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference | $UF_{fish}$ |
|---|---|---|---|---|---|
| Acetaldehyde | 33.85 | 30.80 - 37.20 | 2 | ECOTOX | 0 |
| Acrolein | 0.03 | 0.01 - 0.06 | 8 | ECOTOX | 0 |
| Acrylamide | 117.49 | 109.00 - 124.00 | 3 | ECOTOX | 0 |
| Acrylic acid [1] | 7.90 | | 1 | TOPKAT | 2 |
| Acrylonitrile | 16.90 | 8.40 - 34.00 | 2 | ECOTOX | 0 |
| Ammonia | 6.96 | 5.90 - 8.20 | 2 | ECOTOX | 0 |
| Anthracene | 1.30 | | 1 | TOPKAT ($LC_{50}$ 30x> water solubility) | 3 |
| Benzene | 22.02 | 12.60 - 33.47 | 5 | ECOTOX | 0 |
| Benzoyl peroxide | 3.66 | | 1 | PNN (estimate considered highly uncertain by ESB) | 3 |

| Chemical | 96-hour $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference | $UF_{fish}$ |
|---|---|---|---|---|---|
| Biphenyl | 2.32 | 1.45 - 3.50 | 4 | ECOTOX | 0 |
| Bis(2-ethylhexyl) adipate | 0.001 | | 1 | TOPKAT | 2 |
| Bis(2-ethylhexyl) phthalate | 1106.20 | | 1 | ECOTOX ($LC_{50}$ 3800x > water solubility) | 2 |
| Bromine | | | | No information, default value ($HV_{AAF}$=2.5) | 4 |
| Butadiene:1,3- | 92.10 | | 1 | TOPKAT | 2 |
| Butoxyethanol:2- | 8000.00 | | 1 | TOPKAT | 2 |
| Butyl acrylate | 2.10 | | 1 | TOPKAT | 2 |
| Butyl alcohol:i- | 1484.02 | 1430.00 - 1513.58 | 3 | ECOTOX | 0 |
| Butyl alcohol:n- | 1857.64 | 1730.00 - 1940.00 | 3 | ECOTOX | 0 |
| Butyl alcohol:sec- | 3670.00 | | 1 | ECOTOX | 0 |
| Butyl alcohol:tert- | 6410.00 | | 1 | ECOTOX | 0 |
| Butyl benzyl phthalate | 1.87 | 1.50 - 2.32 | 2 | ECOTOX | 0 |
| Calcium fluoride | 245.99 | 180.00 - 315.00 | 4 | ECOTOX (expressed as fluoride) | 0 |
| Carbon disulphide | 4.00 | | 1 | IUCLID (guppy) | 2 |
| Carbon tetrachloride | 42.53 | 41.40 - 43.30 | 3 | ECOTOX | 0 |
| Chlorine | 0.036 | 0.002 - 1.13 | 13 | ECOTOX<br>IUCLID | 0 |
| Chlorine dioxide | 0.06 | 0.02 - 0.17 | 2 | HSDB | 0 |
| Chlorobenzene | 21.68 | 7.70 - 35.40 | 7 | ECOTOX | 0 |
| Chloroform | 100.90 | 70.70 - 171.00 | 6 | ECOTOX | 0 |
| Chloromethane | 268.28 | | 1 | ECOSAR | 2 |
| Cresol [2] | 12.80 | | 1 | ECOTOX | 0 |
| Cumene | 6.32 | | 1 | ECOTOX | 0 |
| Cumene hydroperoxide | 158.47 | | 1 | OASIS | 2 |
| Cyanides | 0.15 | 0.08 - 0.35 | 37 | ECOTOX (HCN and NaCN) | 0 |
| Cyclohexane | 36.88 | 4.53 117.00 | 5 | ECOTOX | 0 |

| Chemical | 96-hour $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference | $UF_{fish}$ |
|---|---|---|---|---|---|
| Decabromodiphenyl oxide | 735.62 | | 1 | OASIS ($LC_{50}$ 30,000x > water solubility) | 3 |
| Dibutyl phthalate | 1.37 | 0.85 - 3.95 | 7 | ECOTOX | 0 |
| Dichlorobenzene:p- | 8.67 | 2.40 - 34.50 | 10 | ECOTOX | 0 |
| Dichloroethane:1,2- | 125.60 | 116.00 - 136.00 | 2 | ECOTOX | 0 |
| Dichloromethane | 315.53 | 193.00 - 502.00 | 4 | ECOTOX | 0 |
| Dicyclopentadiene | 42.68 | 12.00 - 103.00 | 4 | ECOTOX | 0 |
| Diethanolamine [1] | 1081.60 | 100.00 - 4710.00 | 5 | ECOTOX | 0 |
| Dimethylformamide:n,n- | 10503.05 | 10400.00 - 10600.00 | 3 | ECOTOX | 0 |
| Dioxane:1,4- | 10314.07 | 9850.00 - 10800.00 | 2 | ECOTOX | 0 |
| Di-t-butyl-4-methylphenol:2,6- | 0.25 | | 1 | ASTER | 2 |
| Ethyl acrylate | 2.50 | | 1 | ECOTOX | 0 |
| Ethylbenzene | 21.80 | 9.09 - 48.51 | 4 | ECOTOX | 0 |
| Ethylene | 100.97 | | 1 | ECOSAR | 2 |
| Ethylene glycol | 45633.42 | 8050.00 - 72860.00 | 7 | ECOTOX | 0 |
| Ethylene oxide | 84.00 | | 1 | ECOTOX | 0 |
| Fluorine | | | | No information, default value ($HV_{AAF}$=2.5) | 4 |
| Formaldehyde | 24.10 | | 1 | ECOTOX | 0 |
| Formic acid | 7004.91 | | 1 | ECOSAR | 2 |
| HCFC-141b | 149.40 | | 1 | TOPKAT (HCFC-142b) | 3 |
| HCFC-142b | 149.40 | | 1 | TOPKAT | 2 |
| HCFC-22 | 708.37 | | 1 | ECOSAR | 2 |
| Hexane:n- | 2.50 | | 1 | ECOTOX | 0 |
| Hydrochloric acid | 11.53 | | 1 | IUCLID (bluegill sunfish, pH 3.25, converted to HCl equivalent concentration) | 2 |
| Hydrogen cyanide | 0.14 | 0.12 - 0.16 | 6 | ECOTOX | 0 |
| Hydrogen fluoride | 245.99 | 180.00 - 315.00 | 4 | ECOTOX (expressed as fluoride) | 0 |

| Chemical | 96-hour $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference | $UF_{fish}$ |
|---|---|---|---|---|---|
| Hydrogen sulphide | 0.04 | 0.007 - 0.78 | 27 | ECOTOX | 0 |
| Hydroquinone [1] | 0.04 | | 1 | TOPKAT (experimental database) | 0 |
| Isoprene | 78.80 | 74.83 - 86.51 | 8 | ECOTOX | 0 |
| Isopropyl alcohol | 9246.17 | 6550.00 - 11100.00 | 4 | ECOTOX | 0 |
| Isopropylidenediphenol:p,p'- | 4.65 | 4.60 - 4.70 | 2 | ECOTOX | 0 |
| Lithium carbonate | | | | No information, default value ($HV_{AAF}$=2.5) | 4 |
| Maleic anhydride | 768.00 | | 1 | TOPKAT | 2 |
| Methanol | 28793.75 | 28200.00 - 29400.00 | 2 | ECOTOX | 0 |
| Methyl ethyl ketone | 3220.00 | | 1 | ECOTOX | 0 |
| Methyl isobutyl ketone | 527.09 | 505.00 - 540.00 | 3 | ECOTOX | 0 |
| Methyl methacrylate | 269.29 | 130.00 - 460.00 | 12 | ECOTOX | 0 |
| Methyl tert-butyl ether | 672.00 | | 1 | ECOTOX | 0 |
| Methyl-2-pyrrolidone:N- | 1072.00 | | 1 | IUCLID | 0 |
| Methylenebis (phenylisocyanate) | 1.60 | | 1 | TOPKAT | 2 |
| Naphthalene | 5.10 | 1.99 - 7.90 | 5 | ECOTOX | 0 |
| Nitrate ion [3] | 6000.00 | | 1 | IUCLID ($NaNO_3$, rainbow trout) | 2 |
| Nitric acid | 6.30 | | 1 | HSDB (rainbow trout, pH 4, converted to $HNO_3$ equivalent concentration) | 2 |
| Nitrilotriacetic acid [1] | 82787.46 | | 1 | ASTER ($LC_{50}$ 1.4x > water solubility) | 3 |
| Nonylphenol | 0.16 | 0.128 - 0.270 | 5 | ECOTOX | 0 |
| Phenol [1] | 31.29 | 23.00 - 67.50 | 20 | ECOTOX | 0 |
| Phosphorus [4] | 0.06 | 0.02 - 0.56 | 6 | ECOTOX | 0 |
| Phthalic anhydride | 22.50 | | 1 | TOPKAT | 2 |
| Polymeric diphenylmethane diisocyanate | 1.60 | | 1 | TOPKAT (CAS RN 101-68-8) | 3 |
| Propylene | 178.00 | | 1 | TOPKAT | 2 |
| Sodium fluoride | 245.99 | 180.00 315.00 | 4 | ECOTOX (expressed as fluoride) | 0 |

| Chemical | 96-hour $LC_{50}$ (mg/L) | $LC_{50}$ range | N | Reference | $UF_{fish}$ |
|---|---|---|---|---|---|
| | | - | | | |
| Sodium nitrite | 5.16 | 2.30 - 20.00 | 3 | ECOTOX | 0 |
| Styrene | 21.64 | 4.00 - 59.30 | 6 | ECOTOX | 0 |
| Sulphur hexafluoride | 245.99 | 180.00 - 315.00 | 4 | ECOTOX (expressed as fluoride) | 0 |
| Sulphuric acid | 42.00 | | 1 | IUCLID (mosquito fish) | 2 |
| Tetrachloroethylene | 19.11 | 13.40 - 23.80 | 5 | ECOTOX | 0 |
| Thiourea | > 600 | | 1 | IUCLID | 0 |
| Toluene | 35.62 | 12.60 - 77.40 | 21 | ECOTOX | 0 |
| Toluene-2,4-diisocyanate | 164.50 | | 1 | ECOTOX | 0 |
| Toluenediisocyanate [5] | 164.50 | | 1 | ECOTOX (CAS RN 584-84-9) | 2 |
| Trichloroethylene | 48.20 | 40.70 - 66.80 | 4 | ECOTOX | 0 |
| Triethylamine | 43.70 | | 1 | IUCLID | 0 |
| Trimethylbenzene:1,2,4- | 7.72 | | 1 | ECOTOX | 0 |
| Vinyl acetate | 25.53 | 14.00 - 44.00 | 11 | ECOTOX | 0 |
| Vinyl chloride | 3300.00 | | 1 | TOPKAT | 2 |
| Xylene [5] | 25.64 | 13.40 - 42.00 | 4 | ECOTOX | 0 |

[1] and its salts

[2] mixed isomers and their salts

[3] in solution at pH ≥ 6.0

[4] yellow or white

[5] mixed isomers

***Daphnia magna* 48-hour LC/$EC_{50}$**

| Chemical | 48-hour $EC/LC_{50}$ (mg/L) | $EC/LC_{50}$ range | N | Reference(s) | $UF_{AAD}$ |
|---|---|---|---|---|---|
| Acetaldehyde | 11.67 | 4.7 - 48.25 | 3 | ECOTOX | 0 |
| Acrolein | 0.06 | 0.03 - 0.093 | 5 | ECOTOX | 0 |
| Acrylamide | 160.00 | | 1 | ECOTOX | 0 |
| Acrylic acid [1] | 32.70 | | 1 | TOPKAT | 2 |
| Acrylonitrile | 9.12 | 7.38 - 10.95 | 5 | ECOTOX | 0 |
| Ammonia | 4.18 | | 1 | ECOTOX | 0 |
| Anthracene | 0.22 | 0.036 - 3.03 | 3 | ECOTOX ($EC_{50}$ 5x > water solubility) | 2 |
| Benzene | 93.90 | 9.23 - 682 | 17 | ECOTOX | 0 |
| Benzoyl peroxide | 2.43 | | 1 | ECOSAR | 2 |
| Bis(2-ethylhexyl) adipate | 0.66 | | 1 | ECOTOX | 0 |
| Bis(2-ethylhexyl) phthalate | 4.69 | 2 - 11 | 2 | ECOTOX ($EC/LC_{50}$ 16x > water solubility) | 2 |
| Bromine | 1.00 | | 1 | ECOTOX | 0 |
| Butadiene:1,3- | 40.35 | | 1 | ECOSAR | 2 |
| Butoxyethanol:2- | 22.40 | | 1 | TOPKAT | 2 |
| Butyl acrylate | 9.81 | | 1 | ECOSAR | 2 |
| Butyl alcohol:i- | 1230.54 | 1003 - 1300 | 4 | ECOTOX | 0 |
| Butyl alcohol:n- | 1983.00 | | 1 | ECOTOX | 0 |
| Butyl alcohol:sec- | 4227.00 | | 1 | ECOTOX | 0 |
| Butyl alcohol:tert- | 5504.00 | | 1 | ECOTOX | 0 |
| Butyl benzyl phthalate | 2.85 | 0.62 - 92 | 12 | ECOTOX | 0 |
| Calcium fluoride | 249.59 | 98 - 385 | 8 | ECOTOX | 0 |
| Carbon disulphide | 2.10 | | 1 | ECOTOX | 0 |
| Carbon tetrachloride | 35.00 | | 1 | ECOTOX | 0 |
| Chlorine | 0.09 | 0.017 - 0.15 | 6 | ECOTOX IUCLID | 0 |
| Chlorine dioxide | | | | No information, default value ($HV_{AAD}$=2.5) | 4 |

| Chemical | 48-hour $EC/LC_{50}$ (mg/L) | $EC/LC_{50}$ range | N | Reference(s) | $UF_{AAD}$ |
|---|---|---|---|---|---|
| Chlorobenzene | 11.97 | 0.585 - 86 | 13 | ECOTOX | 0 |
| Chloroform | 98.64 | 51.571 - 758 | 8 | ECOTOX | 0 |
| Chloromethane | 57.00 | | 1 | TOPKAT | 2 |
| Cresol [2] | 5.50 | | 1 | ECOSAR | 2 |
| Cumene | 10.72 | 0.601 - 34.3 | 6 | ECOTOX | 0 |
| Cumene hydroperoxide | 5.14 | | 1 | ECOSAR | 2 |
| Cyanides | 2.19 | 2 - 2.4 | 2 | ECOTOX (KCN) | 0 |
| Cyclohexane | 3.79 | | 1 | ECOTOX | 0 |
| Decabromodiphenyl oxide | 0.00 | | 1 | ECOSAR | 2 |
| Dibutyl phthalate | 3.33 | 2.99 - 3.7 | 2 | ECOTOX | 0 |
| Dichlorobenzene:p- | 8.21 | 2.2 - 13.5 | 5 | ECOTOX | 0 |
| Dichloroethane:1,2- | 306.42 | 160 - 1430 | 7 | ECOTOX | 0 |
| Dichloromethane | 500.63 | 135.808 - 1682 | 4 | ECOTOX | 0 |
| Dicyclopentadiene | 10.50 | | 1 | ECOTOX | 0 |
| Diethanolamine [1] | 115.27 | 55 306 | 11 | ECOTOX | 0 |
| Dimethylformamide:n,n- | 6888.49 | 14.1 - 15700 | 12 | ECOTOX | 0 |
| Dioxane:1,4- | 9040.90 | | 1 | ECOSAR | 2 |
| Di-t-butyl-4-methylphenol:2,6- | 0.08 | | 1 | TOPKAT | 2 |
| Ethyl acrylate | 24.30 | | 1 | ECOSAR | 2 |
| Ethylbenzene | 8.41 | 2.123 - 75 | 6 | ECOTOX | 0 |
| Ethylene | 31.70 | | 1 | TOPKAT | 2 |
| Ethylene glycol | 47347.96 | 41000 - 57600 | 8 | ECOTOX | 0 |
| Ethylene oxide | 201.82 | 137 - 300 | 3 | ECOTOX | 0 |
| Fluorine | | | | No information, default value ($HV_{AAD}$=2.5) | 4 |
| Formaldehyde | 20.58 | 14.6 - 29 | 2 | ECOTOX | 0 |

| Chemical | 48-hour $EC/LC_{50}$ (mg/L) | $EC/LC_{50}$ range | N | Reference(s) | $UF_{AAD}$ |
|---|---|---|---|---|---|
| Formic acid | 151.20 | | 1 | ECOTOX | 0 |
| HCFC-141b | 1.60 | | 1 | TOPKAT (HCFC-142b) | 3 |
| HCFC-142b | 1.60 | | 1 | TOPKAT | 2 |
| HCFC-22 | 37.60 | | 1 | TOPKAT | 2 |
| Hexane:n- | 3.88 | | 1 | ECOTOX | 0 |
| Hydrochloric acid | 56.00 | | 1 | IUCLID (72-hour $LC_{80}$) | 2 |
| Hydrogen cyanide | 2.19 | 2 - 2.4 | 2 | ECOTOX (KCN) | 0 |
| Hydrogen fluoride | 249.59 | 98 - 385 | 8 | ECOTOX | 0 |
| Hydrogen sulphide | | | | Expert judgement ($HV_{AAD}$=5); European chemical Substances Information System datasheet indicates $H_2S$ is very toxic to aquatic organisms. | 2 |
| Hydroquinone [1] | 0.19 | 0.13 - 0.29 | 2 | ECOTOX | 0 |
| Isoprene | 3.20 | | 1 | TOPKAT | 2 |
| Isopropyl alcohol | 1754.09 | | 1 | ECOSAR | 2 |
| Isopropylidenediphenol:p,p'- | 10.20 | | 1 | ECOTOX | 0 |
| Lithium carbonate | | | | No information, default value ($HV_{AAD}$=2.5) | 4 |
| Maleic anhydride | 196.90 | | 1 | TOPKAT | 2 |
| Methanol | 8976.66 | 3289 - 24500 | 2 | ECOTOX | 0 |
| Methyl ethyl ketone | 5091.00 | | 1 | ECOTOX | 0 |
| Methyl isobutyl ketone | 1841.00 | | 1 | TOPKAT (experimental database) | 0 |
| Methyl methacrylate | 69.00 | | 1 | IUCLID | 0 |
| Methyl tert-butyl ether | 622.00 | 542 - 681 | 3 | IUCLID | 0 |
| Methyl-2-pyrrolidone:N- | 4897.00 | | 1 | IUCLID | 0 |
| Methylenebis (phenylisocyanate) | 0.03 | | 1 | TOPKAT | 2 |
| Naphthalene | 5.37 | 1.6 - 22.6 | 12 | ECOTOX | 0 |
| Nitrate ion [3] | 490.00 | | 1 | ECOTOX ($KNO_3$) | 0 |
| Nitric acid | 3581.00 | | 1 | ECOTOX (nitric acid, sodium salt) | 0 |
| Nitrilotriacetic acid [1] | 39.50 | | 1 | TOPKAT (experimental database) | 0 |

| Chemical | 48-hour $EC/LC_{50}$ (mg/L) | $EC/LC_{50}$ range | N | Reference(s) | $UF_{AAD}$ |
|---|---|---|---|---|---|
| Nonylphenol | 0.13 | 0.0848 - 0.19 | 2 | ECOTOX (mixed isomers, CAS# 25154-52-3) | 0 |
| Phenol [1] | 18.51 | 4.2 - 100 | 29 | ECOTOX | 0 |
| Phosphorus (yellow or white) | 0.03 | | 1 | ECOTOX | 0 |
| Phthalic anhydride | 61.40 | | 1 | TOPKAT | 2 |
| Polymeric diphenylmethane diisocyanate | 0.03 | | 1 | TOPKAT | 2 |
| Propylene | 8.10 | | 1 | TOPKAT | 2 |
| Sodium fluoride | 249.59 | 98 - 385 | 8 | ECOTOX | 0 |
| Sodium nitrite | 8.97 | 8.3 - 9.7 | 2 | ECOTOX (96-hour $LC_{50}$) | 2 |
| Styrene | 18.55 | 4.7 - 59 | 3 | ECOTOX | 0 |
| Sulphur hexafluoride | 249.59 | 98 - 385 | 8 | ECOTOX | 0 |
| Sulphuric acid | 29.00 | | 1 | IUCLID (24-hour $EC_{50}$) | 2 |
| Tetrachloroethylene | 10.11 | 7.5 - 18 | 4 | ECOTOX | 0 |
| Thiourea | 9.00 | | 1 | ECOTOX | 0 |
| Toluene | 25.14 | 6 - 310 | 8 | ECOTOX | 0 |
| Toluene-2,4-diisocyanate | 1.50 | | 1 | TOPKAT | 2 |
| Toluenediisocyanate [4] | 12.50 | | 1 | IUCLID | 0 |
| Trichloroethylene | 40.42 | 7.752 - 100 | 8 | ECOTOX | 0 |
| Triethylamine | 200.00 | | 1 | IUCLID | 0 |
| Trimethylbenzene:1,2,4- | 3.61 | | 1 | ECOTOX | 0 |
| Vinyl acetate | 21.20 | | 1 | TOPKAT | 2 |
| Vinyl chloride | 2.70 | | 1 | TOPKAT | 2 |
| Xylene [4] | 0.50 | | 1 | TOPKAT (experimental database) | 0 |

[1] and its salts

[2] mixed isomers and their salts

[3] in solution at pH ≥ 6.0

[4] mixed isomers

## Reaction Half-life

| Chemical | Reaction half-life (days)[1] |
|---|---|
| Acetaldehyde | 1.59 |
| Acrolein | 7.54 |
| Acrylamide | 21.46 |
| Acrylic acid [2] | 3.75 |
| Acrylonitrile | 6.29 |
| Ammonia | 24.33 |
| Anthracene | 11.13 |
| Benzene | 12.96 |
| Benzoyl peroxide | 42.50 |
| Biphenyl | 2.91 |
| Bis(2-ethylhexyl) adipate | 21.83 |
| Bis(2-ethylhexyl) phthalate | 20.04 |
| Bromine | 26.17 |
| Butadiene:1,3- | 0.21 |
| Butoxyethanol:2- | 3.70 |
| Butyl acrylate | 3.70 |
| Butyl alcohol:i- | 2.97 |
| Butyl alcohol:n- | 2.36 |
| Butyl alcohol:sec- | 2.03 |
| Butyl alcohol:tert- | 16.13 |
| Butyl benzyl phthalate | 14.42 |
| Calcium fluoride | 23.63 |
| Carbon disulphide | 3912.50 |
| Carbon tetrachloride | 5208.33 |
| Chlorine | 45.42 |
| Chlorine dioxide | 1262.50 |
| Chlorobenzene | 20.38 |
| Chloroform | 135.83 |
| Chloromethane | 339.58 |
| Cresol [3] | 0.86 |

| Chemical | Reaction half-life (days)[1] |
|---|---|
| Cumene | 2.64 |
| Cumene hydroperoxide | 24.63 |
| Cyanides | 25.42 |
| Cyclohexane | 2.16 |
| Decabromodiphenyl oxide | 217.50 |
| Dibutyl phthalate | 2.85 |
| Dichlorobenzene:p- | 48.33 |
| Dichloroethane:1,2- | 61.67 |
| Dichloromethane | 99.17 |
| Dicyclopentadiene | 0.03 |
| Diethanolamine [2] | 12.50 |
| Dimethylformamide:n,n- | 8.92 |
| Dioxane:1,4- | 18.50 |
| Di-t-butyl-4-methylphenol:2,6- | 52.92 |
| Ethyl acrylate | 0.76 |
| Ethylbenzene | 2.53 |
| Ethylene | 1.52 |
| Ethylene glycol | 12.29 |
| Ethylene oxide | 32.17 |
| Fluorine | 43.75 |
| Formaldehyde | 7.46 |
| Formic acid | 13.50 |
| HCFC-141b | 2550.00 |
| HCFC-142b | 4750.00 |
| HCFC-22 | 2983.33 |
| Hexane:n- | 2.77 |
| Hydrochloric acid | 146.25 |
| Hydrogen cyanide | 172.92 |
| Hydrogen fluoride | 508.33 |
| Hydrogen sulphide | 1337.50 |
| Hydroquinone [2] | 21.67 |

| Chemical | Reaction half-life (days)[1] |
|---|---|
| Isoprene | 0.14 |
| Isopropyl alcohol | 5.17 |
| Isopropylidenediphenol:p,p'- | 54.17 |
| Lithium carbonate | 21.67 |
| Maleic anhydride | 6.71 |
| Methanol | 14.58 |
| Methyl ethyl ketone | 14.58 |
| Methyl isobutyl ketone | 1.35 |
| Methyl methacrylate | 0.82 |
| Methyl tert-butyl ether | 5.42 |
| Methyl-2-pyrrolidone:N- | 20.00 |
| Methylenebis (phenylisocyanate) | 16.71 |
| Naphthalene | 34.17 |
| Nitrate ion [4] | 23.38 |
| Nitric acid | 25.04 |
| Nitrilotriacetic acid [2] | 12.50 |
| Nonylphenol | 19.71 |
| Phenol [2] | 11.96 |
| Phosphorus [5] | 259.58 |
| Phthalic anhydride | 21.67 |
| Polymeric diphenylmethane diisocyanate | 16.71 |
| Propylene | 0.42 |
| Sodium fluoride | 21.67 |
| Sodium nitrite | 21.71 |
| Styrene | 0.31 |
| Sulphur hexafluoride | 5958.33 |
| Sulphuric acid | 21.67 |
| Tetrachloroethylene | 91.67 |
| Thiourea | 21.67 |
| Toluene | 2.97 |
| Toluene-2,4-diisocyanate | 53.75 |

| Chemical | Reaction half-life (days)[1] |
|---|---|
| Toluenediisocyanate [6] | 3.39 |
| Trichloroethylene | 6.63 |
| Triethylamine | 2.00 |
| Trimethylbenzene:1,2,4- | 0.64 |
| Vinyl acetate | 0.69 |
| Vinyl chloride | 2.17 |
| Xylene [6] | 1.69 |

[1] Estimated by Level III fugacity modelling available through EPI Suite v3.12. Note: all reaction half-lives were assigned an uncertainty factor of 2 since they were estimated by the fugacity model.

[2] and its salts

[3] mixed isomers and their salts

[4] in solution at pH ≥ 6.0

[5] yellow or white

[6] mixed isomers

## Log BAF/BCF

| Chemical | Log BAF/BCF | Log BCF Reference | $UF_{BCF}$ | Log Kow used | Log Kow reference |
|---|---|---|---|---|---|
| Acetaldehyde | -1.10 | calculated | 2 | -0.34 | PhysProp |
| Acrolein | 2.54 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Acrylamide | -1.40 | calculated | 2 | -0.67 | PhysProp |
| Acrylic acid [1] | -0.47 | calculated | 2 | 0.35 | PhysProp |
| Acrylonitrile | 1.68 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Ammonia | -2.04 | calculated | 2 | -1.38 | PhysProp |
| Anthracene | 2.81 | log BCF (fathead minnow), Gobas 2000 | 0 | | |
| Benzene | 3.15 | log BCF (striped bass), Gobas 2000 | 0 | | |
| Benzoyl peroxide | 2.36 | calculated | 2 | 3.46 | PhysProp |
| Biphenyl | 2.83 | calculated | 2 | 3.98 | PhysProp |
| Bis(2-ethylhexyl) adipate | 1.43 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Bis(2-ethylhexyl) phthalate | 2.83 | log BAF (pacific staghorn sculpin), Gobas 2000 | 0 | | |
| Bromine | 0.15 | calculated (using QSAR-derived Kow) Inorganic so unlikely to bioaccumulate. | 2 | 1.03 | KOWWIN |
| Butadiene:1,3- | 1.02 | calculated | 2 | 1.99 | PhysProp |
| Butoxyethanol:2- | -0.03 | calculated | 2 | 0.83 | PhysProp |
| Butyl acrylate | 1.36 | calculated | 2 | 2.36 | PhysProp |
| Butyl alcohol:i- | -0.09 | calculated | 2 | 0.76 | PhysProp |
| Butyl alcohol:n- | 0.01 | calculated | 2 | 0.88 | PhysProp |
| Butyl alcohol:sec- | -0.23 | calculated | 2 | 0.61 | PhysProp |
| Butyl alcohol:tert- | -0.47 | calculated | 2 | 0.35 | PhysProp |
| Butyl benzyl phthalate | 4.06 | log BCF (striped seaperch), Gobas 2000 | 0 | | |
| Calcium fluoride | -1.31 | calculated (using QSAR-derived Kow) Inorganic and ionic so unlikely to bioaccumulate. | 2 | -0.58 | KOWWIN |
| Carbon disulphide | 0.98 | calculated | 2 | 1.94 | PhysProp |
| Carbon tetrachloride | 1.48 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Chlorine | -0.01 | calculated (using QSAR-derived Kow) Inorganic gas so unlikely to bioaccumulate. | 2 | 0.85 | KOWWIN |
| Chlorine dioxide | -3.72 | calculated (using QSAR-derived Kow) Inorganic gas so unlikely to bioaccumulate. | 2 | -3.22 | KOWWIN |
| Chlorobenzene | 2.88 | log BAF (blue catfish), Gobas 2000 | 0 | | |

| Chemical | Log BAF/BCF | Log BCF Reference | $UF_{BCF}$ | Log Kow used | Log Kow reference |
|---|---|---|---|---|---|
| Chloroform | 0.78 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Chloromethane | 0.04 | calculated | 2 | 0.91 | PhysProp |
| Cresol [2] | 0.99 | calculated | 2 | 1.95 | PhysProp |
| Cumene | 2.54 | calculated | 2 | 3.66 | PhysProp |
| Cumene hydroperoxide | 1.18 | calculated (using QSAR-derived Kow) | 3 | 2.16 | KOWWIN |
| Cyanide ion | -1.01 | calculated | 2 | -0.25 | PhysProp |
| Cyclohexane | 2.34 | calculated | 2 | 3.44 | PhysProp |
| Decabromodiphenyl oxide | -1.50 | calculated (using QSAR-derived Kow) | 3 | 12.11 | KOWWIN |
| Dibutyl phthalate | 3.13 | log BAF (striped Seaperch), Gobas 2000 | 0 | | |
| Dichlorobenzene:p- | 2.45 | log BAF (spotted sea trout), Gobas 2000 | 0 | | |
| Dichloroethane:1,2- | 0.3 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Dichloromethane | 0.35 | calculated | 2 | 1.25 | PhysProp |
| Dicyclopentadiene | 1.72 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Diethanolamine [1] | -2.09 | calculated | 2 | -1.43 | PhysProp |
| Dimethylformamide:n,n- | -1.71 | calculated | 2 | -1.01 | PhysProp |
| Dioxane:1,4- | -1.03 | calculated | 2 | -0.27 | PhysProp |
| Di-t-butyl-4-methylphenol:2,6- | 3.78 | calculated | 2 | 5.1 | PhysProp |
| Ethyl acrylate | 0.42 | calculated | 2 | 1.32 | PhysProp |
| Ethylbenzene | 2.08 | calculated | 2 | 3.15 | PhysProp |
| Ethylene | 0.24 | calculated | 2 | 1.13 | PhysProp |
| Ethylene glycol | -2.02 | calculated | 2 | -1.36 | PhysProp |
| Ethylene oxide | -1.06 | calculated | 2 | -0.3 | PhysProp |
| Fluorine | -0.59 | calculated (using QSAR-derived Kow)<br>Inorganic gas so unlikely to bioaccumulate. | 2 | 0.22 | KOWWIN |
| Formaldehyde | -0.47 | calculated | 2 | 0.35 | PhysProp |
| Formic acid | -1.28 | calculated | 2 | -0.54 | PhysProp |
| HCFC-141b | 1.31 | calculated | 2 | 2.3 | HSDB |
| HCFC-142b | 1.08 | calculated (using QSAR-derived Kow)<br>Gas at room temperature so unlikely to bioaccumulate. | 2 | 2.05 | KOWWIN |
| HCFC-22 | 0.20 | calculated | 2 | 1.08 | PhysProp |

| Chemical | Log BAF/BCF | Log BCF Reference | $UF_{BCF}$ | Log Kow used | Log Kow reference |
|---|---|---|---|---|---|
| Hexane:n- | 2.76 | calculated | 2 | 3.9 | PhysProp |
| Hydrochloric acid | -0.29 | calculated (using QSAR-derived Kow)<br>Inorganic and ionic so unlikely to bioaccumulate. | 2 | 0.54 | KOWWIN |
| Hydrogen cyanide | -1.01 | calculated | 2 | -0.25 | PhysProp |
| Hydrogen fluoride | -0.58 | calculated (using QSAR-derived Kow)<br>Inorganic gas so unlikely to bioaccumulate. | 2 | 0.23 | KOWWIN |
| Hydrogen sulphide | -2.04 | calculated | 2 | -1.38 | PhysProp |
| Hydroquinone [1] | -0.25 | calculated | 2 | 0.59 | PhysProp |
| Isoprene | 1.42 | calculated | 2 | 2.42 | PhysProp |
| Isopropyl alcohol | -0.74 | calculated | 2 | 0.05 | PhysProp |
| Isopropylidenediphenol:p,p'- | 2.23 | calculated | 2 | 3.32 | PhysProp |
| Lithium carbonate | -1.20 | calculated (using QSAR-derived Kow)<br>Ionic so unlikely to bioaccumulate. | 2 | -0.46 | KOWWIN |
| Maleic anhydride | 0.69 | calculated (using QSAR-derived Kow) | 3 | 1.62 | KOWWIN |
| Methanol | -1.49 | calculated | 2 | -0.77 | PhysProp |
| Methyl ethyl ketone | -0.52 | calculated | 2 | 0.29 | PhysProp |
| Methyl isobutyl ketone | 0.41 | calculated | 2 | 1.31 | PhysProp |
| Methyl methacrylate | 0.47 | calculated | 2 | 1.38 | PhysProp |
| Methyl tert-butyl ether | 0.18 | log BCF (common carp), Gobas 2000 | 0 | | |
| Methyl-2-pyrrolidone:N- | -1.13 | calculated | 2 | -0.38 | PhysProp |
| Methylenebis (phenylisocyanate) | 3.87 | calculated (using QSAR-derived Kow) | 3 | 5.22 | KOWWIN |
| Naphthalene | 3.06 | log BCF (white mullet), Gobas 2000 | 0 | | |
| Nitrate ion [3] | -0.59 | calculated (using QSAR-derived Kow)<br>Inorganic and ionic so unlikely to bioaccumulate. | 2 | 0.21 | KOWWIN |
| Nitric acid | -0.59 | calculated (using QSAR-derived Kow)<br>Inorganic and ionic so unlikely to bioaccumulate. | 2 | 0.21 | KOWWIN |
| Nitrilotriacetic acid [1] | -4.25 | calculated (using QSAR-derived Kow)<br>Inorganic and ionic so unlikely to bioaccumulate. | 2 | -3.81 | KOWWIN |
| Nonylphenol | 2.43 | log BCF (fathead minnow), Gobas 2000 | 0 | | |
| Phenol [1] | 3.67 | log BCF (fathead minnow), Gobas 2000 | 0 | | |
| Phosphorus [4] | -1.03 | calculated (using QSAR-derived Kow)<br>Inorganic so unlikely to bioaccumulate. | 2 | -0.27 | KOWWIN |

| Chemical | Log BAF/BCF | Log BCF Reference | $UF_{BCF}$ | Log Kow used | Log Kow reference |
|---|---|---|---|---|---|
| Phthalic anhydride | 0.67 | calculated | 2 | 1.6 | PhysProp |
| Polymeric diphenylmethane diisocyanate | | Expert judgement ($HV_{BCF}$=1). Not likely to bioaccumulate as substance is a polymer. | 2 | | |
| Propylene | 0.82 | calculated | 2 | 1.77 | PhysProp |
| Sodium fluoride | -0.58 | calculated (using QSAR-derived Kow) Inorganic and ionic so unlikely to bioaccumulate. | 2 | 0.23 | KOWWIN |
| Sodium nitrite | -0.73 | calculated (using QSAR-derived Kow) Inorganic and ionic so unlikely to bioaccumulate. | 2 | 0.06 | KOWWIN |
| Styrene | 1.90 | calculated | 2 | 2.95 | PhysProp |
| Sulphur hexafluoride | 0.74 | calculated | 2 | 1.68 | PhysProp |
| Sulphuric acid | -2.79 | calculated (using QSAR-derived Kow) Inorganic and ionic so unlikely to bioaccumulate. | 2 | -2.2 | KOWWIN |
| Tetrachloroethylene | 1.79 | log BCF (fathead minnow), Gobas 2000 | 0 | | |
| Thiourea | -1.77 | calculated | 2 | -1.08 | PhysProp |
| Toluene | 1.96 | log BCF (fathead minnow), Gobas 2000 | 0 | | |
| Toluene-2,4-diisocyanate | 2.61 | calculated (using QSAR-derived Kow) | 3 | 3.74 | KOWWIN |
| Toluenediisocyanate [5] | 2.61 | calculated (using QSAR-derived Kow) | 3 | 3.74 | KOWWIN |
| Trichloroethylene | 1.23 | log BCF (bluegill sunfish), Gobas 2000 | 0 | | |
| Triethylamine | 0.53 | calculated | 2 | 1.45 | PhysProp |
| Trimethylbenzene:1,2,4- | 2.51 | calculated | 2 | 3.63 | PhysProp |
| Vinyl acetate | -0.12 | calculated | 2 | 0.73 | PhysProp |
| Vinyl chloride | 0.69 | calculated using QSAR-derived Kow | 3 | 1.62 | KOWWIN |
| Xylene [5] | 2.05 | calculated | 2 | 3.12 | PhysProp |

[1] and its salts

[2] mixed isomers and their salts

[3] in solution at pH ≥ 6.0

[4] yellow or white

[5] mixed isomers