

Development of the Alternatives Assessment Dashboard

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US EPA Disclaimer

- *“The views expressed in this presentation are those of the author[s] and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.”*

Alternatives Assessment

- The goal of alternatives assessment is to identify safer alternatives for chemicals of concern.

Alternatives Assessment Dashboard

- Hazard profiles compare alternatives in terms of Low, Medium, High, and Very High (L, M, H, VH) scores for a variety of categories
- Categories include

Acute mammalian toxicity*	Reproductive toxicity	Skin sensitization
Carcinogenicity	Developmental toxicity*	Eye and skin irritation
Mutagenicity*	Neurotoxicity	Acute* and chronic aquatic toxicity
Endocrine disruption*	Systemic toxicity	Persistence and bioaccumulation*

- Data from quantitative toxicity values, GHS scores, QSAR models, government lists

Alternatives Assessment Dashboard.

➤ Compare alternatives in terms of color-coded comparison table of
L, M, H, VH scores

Structure CAS name	Human Health Effects															Ecotoxicity		Fate	
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure							
79-01-6 Trichloroethylene	L	M	L	VH	H	N/A	H	H	N/A	N/A	H	M	N/A	H	H	M	M	H	L
127-18-4 Perchloroethylene	L	L	N/A	VH	L	H	N/A	L	N/A	N/A	M	M	N/A	H	H	M	H	H	L
81-33-4 Pigment Violet 29	M	N/A	N/A	N/A	H	N/A	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	L	M	H	L
872-50-4 N-ethylpyrrolidone	L	N/A	L	N/A	L	L	H	H	N/A	N/A	N/A	M	N/A	H	H	L	N/A	L	L
123-91-1 1,4-dioxane	M	L	L	VH	H	L	N/A	L	N/A	N/A	M	M	N/A	M	H	L	N/A	H	L
106-94-5 1-Bromopropane	M	L	N/A	VH	L	L	H	H	N/A	N/A	M	M	N/A	H	H	M	N/A	H	L
56-23-5 Carbon tetrachloride	H	H	H	VH	L	H	N/A	L	N/A	N/A	H	H	H	H	H	VH	M	H	L
1332-21-4 Asbestos	N/A	N/A	N/A	VH	N/A	N/A	N/A	N/A	N/A	N/A	H	N/A	N/A	N/A	N/A	L	N/A	H	L
75-09-2 Methylene chloride	M	L	N/A	VH	H	H	N/A	H	N/A	N/A	M	H	N/A	H	H	L	N/A	H	L
25637-99-4 Hexabromocyclododecane	M	N/A	N/A	N/A	H	H	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	VH	VH	N/A	L
3194-55-6 1,2,5,6,9,10-Hexabromocyclododecane	L	N/A	N/A	N/A	H	H	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	VH	VH	H	H
3194-57-8 1,2,5,6-Tetrabromocyclooctane	L	N/A	N/A	N/A	H	L	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	VH	N/A	N/A	M

Sources of alternative assessment scores

- Quantitative data
 - US EPA Chemistry Dashboard / RapidTox , Chemidplus
- QSAR Predictions
 - WebTEST
- GHS data
 - Australia, Canada, Denmark, ECHA, Japan, Korea, Malaysia, New Zealand, Germany
- Lists
 - DSL, EPA Mid Atlantic Human Health, Health Canada Priority Substance Lists Carcinogenicity, Health Canada Priority Substance Lists Reproductive, IARC, IRIS, NIOSH Potential Occupational Carcinogens, Prop65, Reach Very High Concern List, Report On Carcinogens, SIN, TEDX, TSCA Work Plan, UMD
- Future work
 - QSAR/read across models based on compiled experimental values
 - Quantitative data from REACH dossiers

WebTEST on EPA's Chemistry Dashboard

Chemistry Dashboard

Aa ▼ Aa Aa ▲

Predictions

Q 91-20-3

×

100%

⚙️ ? ⓘ

Select properties to predict

T.E.S.T. 18

☒ Toxicological properties + -

- ☒ 96 hour fathead minnow LC50
- ☒ 48 hour D. magna LC50
- ☒ 48 hour T. pyriformis IGC50
- ☒ Oral rat LD50
- ☒ Bioaccumulation factor
- ☒ Developmental toxicity
- ☒ Ames mutagenicity
- ☒ Estrogen Receptor RBA
- ☒ Estrogen Receptor Binding

☒ Physical properties + -

- ☒ Normal boiling point
- ☒ Melting point
- ☒ Flash point
- ☒ Vapor pressure
- ☒ Density
- ☒ Surface tension
- ☒ Thermal conductivity
- ☒ Viscosity
- ☒ Water solubility

Calculate

<https://comptox.epa.gov/dashboard/predictions/index>

WebTEST GUI output

← → ↻ ⓘ Not secure | comptox.ag.epa.gov/dashboard/predictions/index

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Search All Data 🔍

Chemistry Dashboard

Aa Aa Aa ▲

Predictions

Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50	4.320 -Log10(mol/L) 6.135 mg/L	4.221 -Log10(mol/L) 7.710 mg/L	4.197 -Log10(mol/L) 8.148 mg/L	4.012 -Log10(mol/L) 12.482 mg/L	4.242 -Log10(mol/L) 7.347 mg/L	4.433 -Log10(mol/L) 4.730 mg/L
48 hour D. magna LC50	4.147 -Log10(mol/L) 9.137 mg/L	4.237 -Log10(mol/L) 7.422 mg/L	4.137 -Log10(mol/L) 9.355 mg/L	4.130 -Log10(mol/L) 9.503 mg/L	4.264 -Log10(mol/L) 6.972 mg/L	4.418 -Log10(mol/L) 4.896 mg/L
48 hour T. pyriformis IGC50	2.880 -Log10(mol/L) 168.974 mg/L	3.411 -Log10(mol/L) 49.758 mg/L	3.092 -Log10(mol/L) 103.622 mg/L		3.574 -Log10(mol/L) 34.197 mg/L	3.567 -Log10(mol/L) 34.766 mg/L
Oral rat LD50	2.418 -Log10(mol/kg) 489.576 mg/kg	2.114 -Log10(mol/kg) 985.677 mg/kg	2.146 -Log10(mol/kg) 916.183 mg/kg			2.082 -Log10(mol/kg) 1060.442 mg/kg
Bioaccumulation factor	2.360 Log10 229.086	2.351 Log10 224.335	2.368 Log10 233.308	2.511 Log10 324.522	2.011 Log10 102.507	2.514 Log10 326.333
Developmental toxicity		false	true	false		false
Ames mutagenicity	false					false
Estrogen Receptor RBA		-5.225 Log10 5.95*10 ⁻⁶	-6.438 Log10 3.646*10 ⁻⁷	-6.438 Log10 3.646*10 ⁻⁷		-2.800 Log10 0.002

Scores from T.E.S.T predictions

Chemical	Oral rat LD50 mg/kg	Fathead minnow LC50 mg/L	Dev. Tox.	Mutage nicity	Acute Mammalian Tox Score	Acute Aquatic Tox Score	Dev. Tox. Score	Mutageni city Score
DecaBDE	>5000 ^e	6.44E-04	N/A	— ^e	L	L*	N/A	L
TPP	3496 ^e	9.30E-01 ^e	+	— ^e	L	VH	H	L
RDP	2216	3.15E-02	N/A	—	L	VH	N/A	L
BPADP	2261	7.30E-01	N/A	—	L	L*	N/A	L

*Toxicity value exceeds water solubility so score is “L”

Counts from other sources

Source	Acute Mammalian Toxicity Oral	Acute Mammalian Toxicity Inhalation	Acute Mammalian Toxicity Dermal	Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity Repeat Exposure	Neurotoxicity Single Exposure	Systemic Toxicity Repeat Exposure	Systemic Toxicity Single Exposure	Skin Sensitization	Eye Irritation	Skin Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
Australia	352	459	127	509	315	0	217	340	0	0	378	71	172	277	396	54	44	0	0
Canada	407	236	131	263	71	0	135	135	0	0	246	196	180	391	434	0	0	0	0
ChemIDplus	29110	1239	3081	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Denmark	15224	0	0	3726	5742	0	4036	0	0	0	0	0	9668	0	8008	3619	14160	0	0
DSL	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20127	0	20981	20603
ECHA CLP	1612	761	623	1235	627	0	202	299	0	0	636	338	1168	997	953	1262	2428	0	0
EPA mid-Atlantic Region Human Health Risk-Based Concentrations	0	0	0	217	29	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Germany	0	0	0	398	81	0	0	300	0	0	0	0	262	0	0	0	0	0	0
Health Canada Priority Substance Lists (Carcinogenicity)	0	0	0	151	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Health Canada Priority Substance Lists (Reproductive Toxicity)	0	0	0	0	0	0	38	0	0	0	0	0	0	0	0	0	0	0	0
IARC	0	0	0	511	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
IRIS	0	0	0	126	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Japan	2200	890	1300	764	858	0	961	963	536	703	1241	1262	740	1714	1599	1338	1343	0	0
Malaysia	130	118	91	58	24	0	15	16	0	0	42	63	34	103	81	79	77	0	0
New Zealand	4356	1489	1112	697	412	0	1253	0	0	0	1883	0	0	4663	4076	0	3655	0	0
NIOSH list of potential occupational carcinogens	0	0	0	133	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Prop 65	0	0	0	617	0	0	40	291	0	0	0	0	0	0	0	0	0	0	0
REACH Very High Concern List	0	0	0	81	22	5	104	0	0	0	7	0	0	0	0	0	0	38	38
Report On Carcinogens	0	0	0	272	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SIN	0	0	0	0	0	112	0	0	0	0	0	0	0	0	0	0	0	0	0
TEDX	0	0	0	0	0	1292	0	0	0	0	0	0	0	0	0	0	0	0	0
TSCA work plan	5	8	0	36	4	0	15	12	4	0	3	0	0	0	0	8	9	90	90
UMD	437	0	0	349	859	0	0	0	0	0	0	0	0	0	0	0	0	0	0
All sources (unique CAS)	44903	3365	4480	6633	8264	1348	6311	1837	539	703	3495	1523	11527	6345	13234	24328	19975	21023	20647

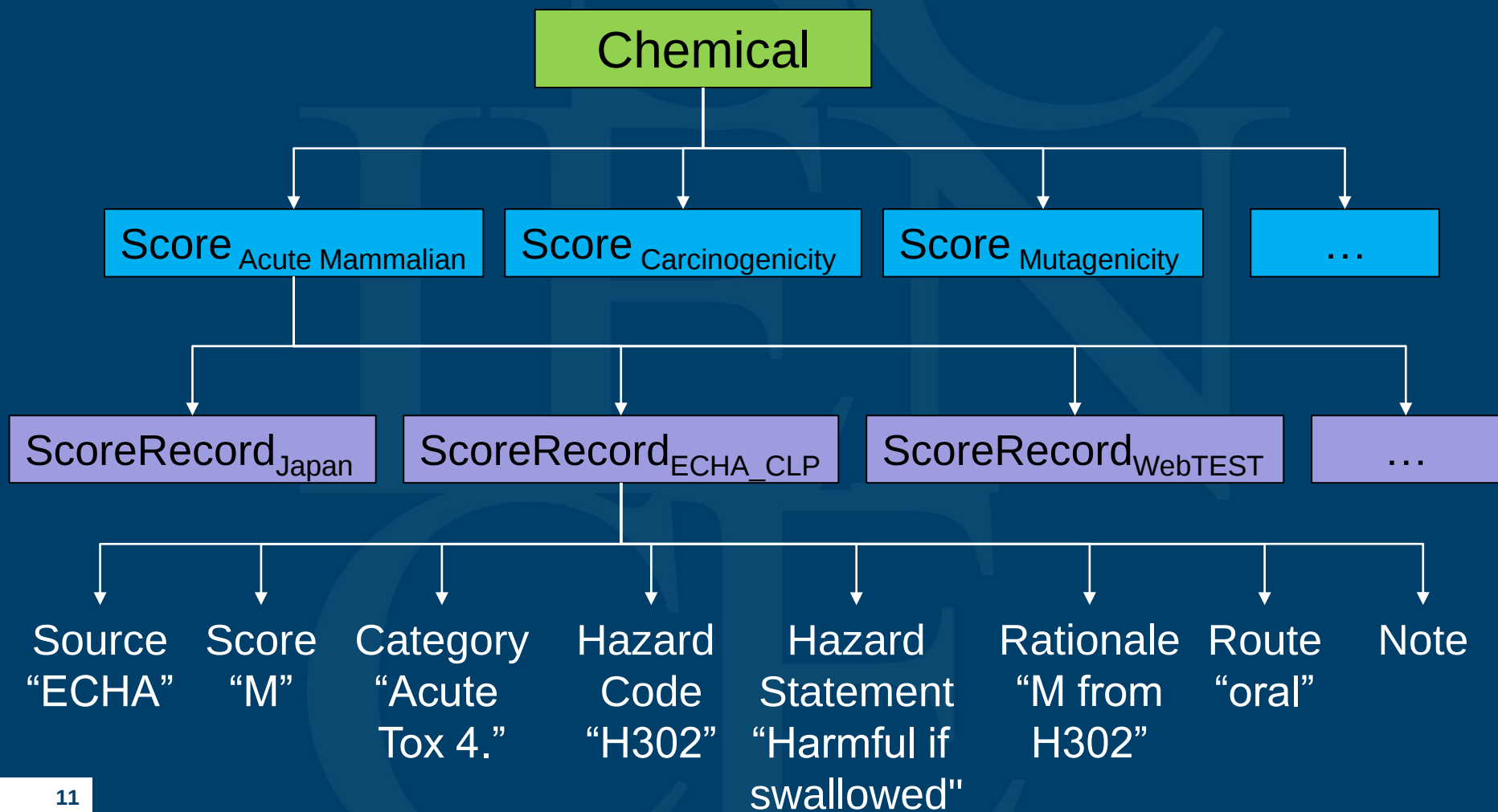
Converting between systems

Acute toxicity scoring

Risk phrase	R28	R25			R22		
LD50, mg/kg	≤5	5-25	25-50	50-200	200-300	300-2000	2000-5000
GHS	Cat 1	Category 2	Category 3		Category 4	Category 5	
EU CLP	H300		H301		H302	H303	
DfE Score	Very high		High		Moderate	Low	

➤ Quantitative toxicity scores are preferable due to differing systems

AA Data Class Structure



Assigning the final score

➤ Trumping Scheme

- Predicted score is the most toxic score from the source with the highest authority
- Authority levels include Authoritative (e.g. ECHA CLP), Screening (e.g. Chemidplus), and Predicted (e.g. WebTEST)

➤ Weighted average

- Predicted score is the weighted average from the different sources:

$$score_{final} = \frac{\sum_{i=1}^{\#sources} score_i w_i}{\sum_{i=1}^{\#sources} w_i}$$

- $score_{final}$ is rounded to nearest integer and converted to qualitative score (L=1, M=2, etc.)
- $w_i = 10, 5$, and 1 for Authoritative, Screening, and Predicted, respectively

Mockup of AA Dashboard (batch mode of WebTEST)

Dashboard Search

Select Input Type(s)

☐ Chemical Name 
☐ CASRN 
☐ InChIKey  ☐ Skeleton 
☐ DSSTox Substance ID 
☐ MS-Ready Formula(e) 
☐ Exact Formula(e) 
☐ Monoisotopic Mass 

Enter identifiers to Search

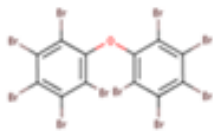
71-43-2
91-20-3

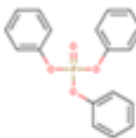
Search

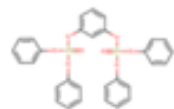
Draw...

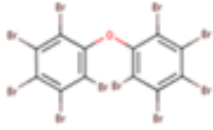
SDF File...

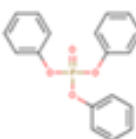
Selected Chemicals

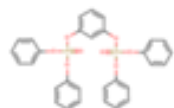

1163-19-5


115-86-6


57583-54-7


1163-19-5


115-86-6


57583-54-7

Endpoint:

Fathead minnow LC50 (96 hr)

Calculate

Alternatives Assessment:

Generate

AA Dashboard output

Structure CAS name	Human Health Effects															Ecotoxicity		Fate	
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure							
79-01-6 Trichloroethylene	L	M	L	VI	H	N/A	H	H	N/A	N/A	H	M	N/A	H	H	M	M	H	L
127-18-4 Perchloroethylene	L	L	N/A	VI	L	H	N/A	L	N/A	N/A	M	M	N/A	H	H	M	H	H	L
81-33-4 Pigment Violet 29	M	N/A	N/A	N/A	H	N/A	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	L	M	H	L
872-50-4 N-ethyl-methylpyrrolidone	L	N/A	L	N/A	L	L	H	H	N/A	N/A	N/A	M	N/A	H	H	L	N/A	L	L
123-91-1 1,4-dioxane	M	L	L	VI	H	L	N/A	L	N/A	N/A	M	M	N/A	M	H	L	N/A	H	L
106-94-5 1-Bromopropane	M	L	N/A	VI	L	L	H	H	N/A	N/A	M	M	N/A	H	H	M	N/A	H	L
56-23-5 Carbon tetrachloride	H	H	H	VI	L	H	N/A	L	N/A	N/A	H	H	H	H	H	VI	M	H	L
1332-21-4 Asbestos	N/A	N/A	N/A	VI	N/A	N/A	N/A	N/A	N/A	N/A	H	N/A	N/A	N/A	N/A	L	N/A	H	L
75-09-2 Methylene chloride	M	L	N/A	VI	H	H	N/A	H	N/A	N/A	M	H	N/A	H	H	L	N/A	H	L
25637-99-4 Hexabromocyclododecane	M	N/A	N/A	N/A	H	H	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	VI	VI	N/A	L
3194-55-6 1,2,5,6,9,10-Hexabromocyclododecane	L	N/A	N/A	N/A	H	H	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	VI	VI	H	H
3194-57-8 1,2,5,6-Tetrabromocyclooctane	L	N/A	N/A	N/A	H	L	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	VI	N/A	N/A	M

Structure CAS name	Human Health Effects															Ecotoxicity		Fate	
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure							
79-01-6 Trichloroethylene	L	M	L	M	M	N/A	H	H	H	H	H	M	H	H	H	M	M	H	L
127-18-4 Perchloroethylene	L	M	L	M	L	H	M	L	H	H	H	H	N/A	H	H	M	H	H	L
81-33-4 Pigment Violet 29	M	N/A	N/A	N/A	H	N/A	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	L	M	H	L
872-50-4 N-ethylpyrrolidone	L	L	L	N/A	L	L	H	H	M	N/A	M	M	N/A	H	H	L	L	L	L
123-91-1 1,4 - dioxane	M	M	L	M	M	L	N/A	L	H	H	H	M	N/A	H	H	L	L	H	L
106-94-5 1 - Bromopropane	L	M	L	M	L	L	H	H	H	N/A	M	M	N/A	H	H	M	M	H	L
56-23-5 Carbon tetrachloride	H	H	H	M	L	H	M	L	Trumping					H	H	M	M	H	L
1332-21-4 Asbestos	N/A	N/A	N/A	M	H	N/A	N/A	N/A						N/A	L	N/A	H	L	
75-09-2 Methylene chloride	M	M	N/A	M	M	H	M	H	H	H	H	H	N/A	H	H	L	N/A	H	L
25637-99-4 Hexabromocyclododecane	L	L	L	N/A	H	H	M	H	N/A	N/A	N/A	M	L	L	L	M	M	N/A	L
3194-55-6 1,2,5,6,9,10- Hexabromocyclododecane	L	N/A	N/A	N/A	H	H	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	M	M	H	H
3194-57-8 1,2,5,6-Tetrabromocyclooctane	L	N/A	N/A	N/A	H	L	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	M	N/A	N/A	M

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79-01-6 Trichloroethylene	L	M	L	M	H	N/A	H	H	H	H	M	M	H	H	H	M	M	H	L
127-18-4 Perchloroethylene	L	L	L	M	L	H	M	M	H	H	M	H	N/A	H	H	M	H	H	L
81-33-4 Pigment Violet 29	M	N/A	N/A	N/A	H	N/A	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	L	M	H	L
872-50-4 N-ethyl-2-pyrrolidone	L	L	L	N/A	L	L	H	H	M	N/A	M	M	N/A	H	H	L	L	L	L
123-91-1 1,4-dioxane	L	L	L	M	M	L	N/A	L	H	H	M	M	N/A	H	H	L	L	M	L
106-94-5 1-Bromopropane	L	M	L	M	L	L	H	H	H	N/A	M	M	N/A	H	H	M	M	M	L
56-23-5 Carbon tetrachloride	M	M	M	M	L	H	M	H	Weighted Average					H	H	M	M	H	L
1332-21-4 Asbestos	N/A	N/A	N/A	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	L	N/A	H	L
75-09-2 Methylene chloride	M	L	N/A	M	M	H	M	H	H	H	M	H	N/A	H	H	L	N/A	M	L
25637-99-4 Hexabromocyclododecane	L	L	L	N/A	H	H	M	H	N/A	N/A	N/A	M	L	L	L	M	M	N/A	L
3194-55-6 1,2,5,6,9,10-Hexabromocyclododecane	L	N/A	N/A	N/A	H	H	M	H	N/A	N/A	N/A	N/A	N/A	N/A	N/A	M	M	H	H
3194-57-8 1,2,5,6-Tetrabromocyclooctane	L	N/A	N/A	N/A	H	L	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	M	N/A	N/A	M

* ~12% are different (omitting N/A scores)

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Records for Acute Mammalian Toxicity Oral for 56-23-5

Score records sorted by Authority (descending), Score (descending), and Source (ascending)

Source	Authority	Score	Route	Category	Hazard Code	Hazard Statement	Rationale	Note
ECHA CLP	Authoritative	H	oral	Acute Tox. 3	H301	Toxic if swallowed	Score of H was assigned based on a hazard code of H301	
UMD	Screening	VH		Acute toxin			Score of VH was assigned based on a category of Acute toxin	Meets the University of Maryland definition of an "Acute Toxin" for the purpose of the University of Maryland Chemical Hygiene Plan. Acute toxins are defined as substances that have a median lethal dose (LD50) less than or equal to 50 mg/kg body weight by the oral route of entry; 200 mg/kg body weight by the dermal route of entry or a median lethal concentration (LC50) less than or equal to 0.5 mg/l where time of exposure is eight hours or less. This definition is compatible with the 1994 Department of Transportation definition of "Poison".
Korea	Screening	H	oral		H301	Toxic if swallowed	Score of H was assigned based on a hazard code of H301	
New Zealand	Screening	H	oral	Category 6.1C (Category 3)		Acutely toxic	Score was assigned based on a category of Category 6.1C (Category 3).	R-PHRASE: R 25 [N-CLASS]
ChemIDplus	Screening	L	Oral				Oral LD50(5760 mg/kg) > 2000 mg/kg	Test organism: guinea pig Reported Dose: 5760mg/kg Normalized Dose: 5760mg/kg Source: Gigiena i Sanitariya. For English translation, see HYSAAV. Vol. 33(1), Pg. 32, 1968.
ChemIDplus	Screening	L	Oral				Oral LD50(8263 mg/kg) > 2000 mg/kg	Test organism: mouse Reported Dose: 8263mg/kg Normalized Dose: 8263mg/kg Source: Journal of Pharmacy and Pharmacology. Vol. 3, Pg. 169, 1951.
ChemIDplus	Screening	L	Oral				Oral LD50(5760 mg/kg) > 2000 mg/kg	Test organism: rabbit Reported Dose: 5760mg/kg Normalized Dose: 5760mg/kg
ChemIDplus	Screening	L	Oral				Oral LD50(5760 mg/kg) > 2000 mg/kg	Test organism: rabbit Reported Dose: 5760mg/kg Normalized Dose: 5760mg/kg
ChemIDplus	Screening	L	Oral				Oral LD50(5760 mg/kg) > 2000 mg/kg	Test organism: rabbit Reported Dose: 5760mg/kg Normalized Dose: 5760mg/kg Source: Gigiena i Sanitariya. For English translation, see HYSAAV. Vol. 33(1), Pg. 32, 1968.
ChemIDplus	Screening	L	Oral				Oral LD50(2350 mg/kg) > 2000 mg/kg	Test organism: rat Reported Dose: 2350mg/kg Normalized Dose: 2350mg/kg Source: Archives of Toxicology. Vol. 54, Pg. 275, 1983.
Japan	Screening	L	oral	Category 5		May be harmful if swallowed	Score was assigned based on a category of "Category 5".	Based on the LD50 value of 2,350mg/kg calculated from the testing data of rat LD50 (oral route) of 2,350mg/kg (MOE Risk Assessment Vol. 1, 2002), 2,821mg/kg and 10,054mg/kg (EHC 208, 1999).
T.E.S.T. (predicted value)	QSAR Model	L	Oral				Oral rat LD50 (2145 mg/kg) > 2000 mg/kg	

Questions???