

Generation of GHS Scores from TEST and online sources

Todd Martin, US EPA

Sources of scores

➤ US EPA

- Chemistry Dashboard: <http://comptox.ag.epa.gov/dashboard>
 - ACToR/ToxRefDB
- T.E.S.T. (Toxicity Estimation Software Tool)

➤ ECHA (European Chemicals Agency)

- REACH dossiers / Hazard statement codes

➤ ChemHAT

- Free compilation of data from EU (both R and H scores), New Zealand, Australia, Japan (NITE), Korea, Malaysia, and miscellaneous lists

➤ Wehage developed a system to assign scores from Japan's NITE data

➤ Future work

- QSAR/read across models based on compiled experimental values

Converting between systems

Acute toxicity scoring

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

➤ Quantitative toxicity scores are preferable due to differing systems



T.E.S.T (Toxicity Estimation Software Tool)

File Edit Help

Predicted Fathead minnow LC50 (96 hr) for 71-43-2

Prediction results

Endpoint	Experimental value (CAS= 71-43-2) Source: ECOTOX
Fathead minnow LC ₅₀ (96 hr) -Log10(mol/L)	3.44
Fathead minnow LC ₅₀ (96 hr) mg/L	28.04

^aNote: the test chemical was present in the training set. The prediction does not

Individual Predictions	
Method	Predicted value -Log10(mol/L)
Hierarchical clustering	3.46
Single model	3.19
Group contribution	2.95
Nearest neighbor	3.51

Test chemical

Descriptor values for test chemical

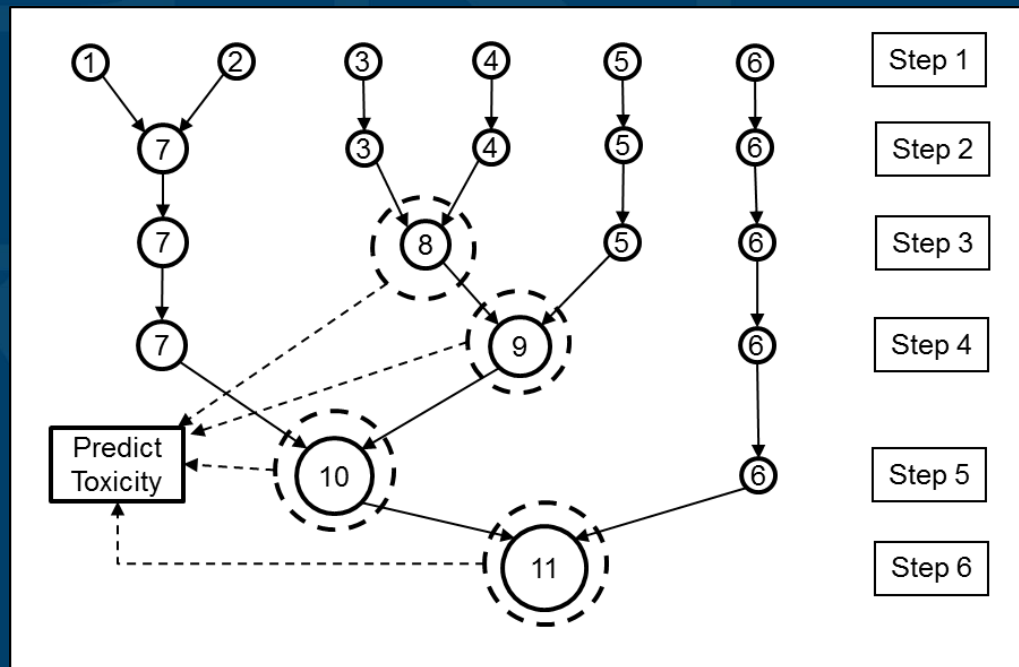
Draw a structure or enter a CAS number (i.e. 71-43-2) in the Molecule ID field and click "Enter structure". A Molecule ID is required for file output.

Molecule ID: Enter structure
 Endpoint: Fathead minnow LC50 (96 hr) ?
 Method: Consensus ?

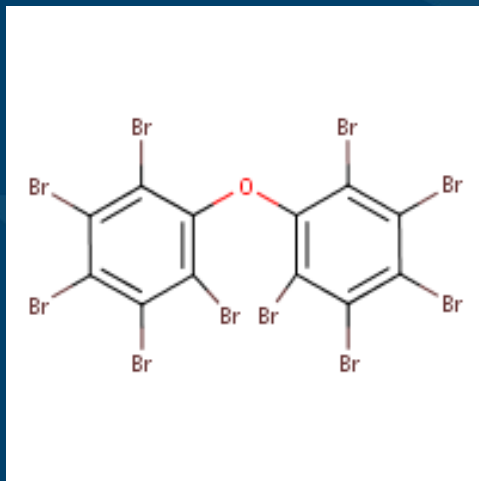
Options...
Calculate

QSAR Methods

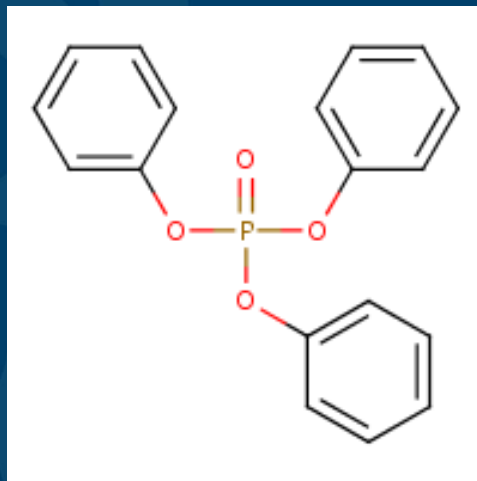
- Hierarchical clustering
- Single Model
- Group contribution
- Nearest neighbor
- Consensus



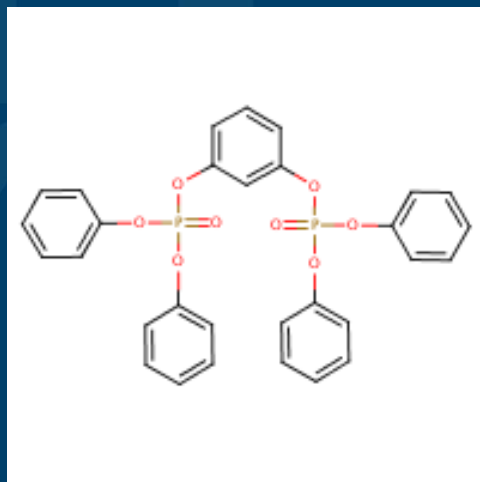
Case Study: flame retardant alternatives and their metabolites



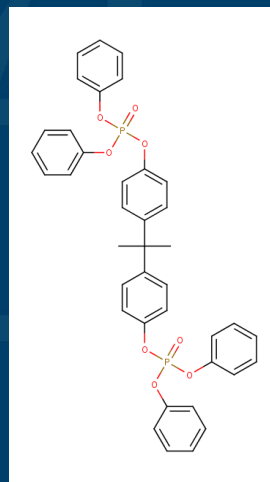
DecaBDE



TPP



RDP



BPADP

Physical properties from T.E.S.T.

Name	MP*, ° C	BP, ° C	FP, ° C	VP, mmHg
DecaBDE	295 ^e	530 ^e	241 ^e	3.01E-12
TPP	51 ^e	381	201 ^e	6.28E-06 ^e
RDP	87	446	307	4.76E-08
BPADP	114	435	378 ^e	4.21E-10

^e experimental value

- MP, BP: indicate state of matter
- VP: inhalation implications
- FP: flammability

Water based properties from T.E.S.T

Name	WS, mg/L	log Kow	log BCF	Bioacc. score
DecaBDE	1.00E-04 ^e	12.11	1.20 ^e	L
TPP	1.90E+00 ^e	4.70	2.48 ^e	M
RDP	2.90E-01	7.41	1.82	L
BPADP	9.19E-02	10.02	1.28	L

^e experimental value

- WS: aquatic toxicity implications
- LogKow: can be used to estimate partitioning
- BCF: bioaccumulation in fish

Human health hazards and ecotoxicity values from T.E.S.T

Chemical	Oral rat LD50 mg/kg	Fathead minnow LC50 mg/L	Dev. Tox.	Mutagenicity	Acute Mammalian Tox Score	Acute Aquatic Tox Score	Dev. Tox. Score	Mutagenicity Score
DecaBDE	>5000 ^e	6.44E-04	N/A	— ^e	L	VH*	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	VH*	N/A	L

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

T.E.S.T. (Toxicity Estimation Software Tool)

- Currently T.E.S.T. is available as a downloadable standalone Java application
- In 2017, T.E.S.T. will be converted to a web-services based application which will allow predictions on the CompTox dashboard
 - <http://comptox.ag.epa.gov/dashboard/>
- Predictions using T.E.S.T. models for 743,000 chemicals are now being stored within the CompTox dashboard

Chemistry Dashboard

Submit Comment

Copy ▾

Aa ▾

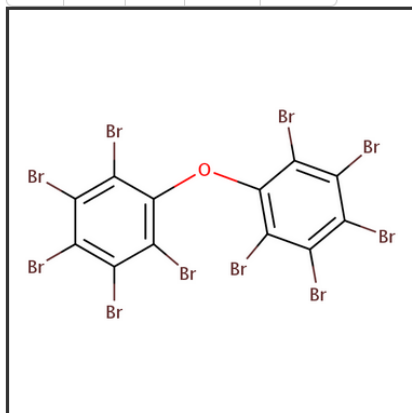
Aa

Aa ▴

BDE-209

1163-19-5 | DTXSID9020376

© Searched by CAS-RN: Found 1 result for
'1163-19-5'.



Wikipedia

Decabromodiphenyl ether (also known as decaBDE, deca-BDE, DBDE, deca, decabromodiphenyl oxide, DBDPO, or bis(pentabromophenyl) ether) is a brominated flame retardant which belongs to the group of polybrominated diphenyl ethers (PBDEs).... [Read more](#)

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

Chemistry Dashboard, cont.

Chemical Properties	Synonyms	External Links	Env. Fate/Transport	Toxicity Values (Beta)	Bioassays	Exposure	Literature
Similar Molecules (Beta)	Comments						

Summary

Download as: TSV Excel SDF

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-	9.60 (4)	-	9.60	-	7.36 to 12.1	-
Water Solubility	-	2.27e-08 (4)	-	2.27e-08	-	2.96e-17 to 9.09e-08	mol/L
Density	-	2.98 (1)	-	2.98	-	-	g/cm ³
Melting Point	304 (5)	290 (3)	306	290	304 to 308	255 to 313	°C
Boiling Point	530 (1)	540 (3)	530	540	530	509 to 590	°C
Surface Tension	-	62.0 (1)	-	62.0	-	-	dyn/cm
Vapor Pressure	-	1.01e-11 (3)	-	1.01e-11	-	1.64e-12 to 2.57e-11	mmHg
LogKoa: Octanol-Air	-	11.7 (1)	-	11.7	-	-	-
Henry's Law	-	5.67e-04 (1)	-	5.67e-04	-	-	atm-m ³ /mole
Index of Refraction	-	1.74 (1)	-	1.74	-	-	-
Molar Refractivity	-	130 (1)	-	130	-	-	cm ³
Molar Volume	-	322 (1)	-	322	-	-	cm ³
Polarizability	-	51.4 (1)	-	51.4	-	-	Å ³

[Chemical Properties](#)
[Synonyms](#)
[External Links](#)
[Env. Fate/Transport](#)
[Toxicity Values \(Beta\)](#)
[Bioassays](#)
[Exposure](#)
[Literature](#)
[Similar Molecules \(Beta\)](#)

General

- [EPA Substance Registr...](#)
- [NIST Chemistry Webbook](#)
- [Household Products D...](#)
- [PubChem](#)
- [Chemspider](#)
- [CPCat](#)
- [Wikipedia](#)
- [MSDS Lookup](#)
- [ToxPlanet](#)
- [ChemHat Hazards and...](#)
- [ChEMBL](#)
- [Chemical Vendors](#)
- [Consumer Product Info...](#)
- [Sigma-Aldrich Chemicals](#)
- [Wikidata](#)
- [Wolfram Alpha](#)
- [WebWISER](#)
- [ChemAgora](#)
- [ECHA Infocard](#)
- [ECHA Brief Profile](#)
- [ScrubChem](#)
- [ECHA Dossier](#)

Toxicology

- [ACToR](#)
- [DrugPortal](#)
- [CCRIS](#)
- [ChemView](#)
- [CTD](#)
- [eChemPortal](#)
- [EDSP Dashboard](#)
- [Gene-Tox](#)
- [HSDB](#)
- [ToxCast Dashboard 2](#)
- [LactMed](#)
- [International Toxicity Es...](#)
- [ACToR PDF Report](#)

Publications

- [Toxline](#)
- [Environmental Health P...](#)
- [NIEHS](#)
- [National Toxicology Pro...](#)
- [Google Books](#)
- [Google Scholar](#)
- [Google Patents](#)
- [PubMed](#)
- [BioCaddie DataMed](#)
- [Federal Register](#)
- [Regulations.gov](#)
- [RSC Publications](#)
- [Springer Materials](#)
- [IRIS Assessments](#)
- [CORE Literature Search](#)
- [Bielefeld Academic Se...](#)

Analytical

- [RSC Analytical Abstracts](#)
- [FOR-IDENT](#)
- [MONA: MassBank Nort...](#)
- [NEMI: National Environ...](#)

Prediction

- [Chemicalize](#)
- [Proton NMR Prediction](#)
- [Carbon-13 NMR Predic...](#)
- [2D NMR HSQC/HMBC ...](#)
- [ChemRTP Predictor](#)

Acute Toxicity

Show Data Hide Data

- ▶  CheLIST combination of files from EU Research lists
- ▶  EPA IRIS (Integrated Risk Information System)
- ▶  INCHEM Environmental Health Criteria Monographs
- ▶  INCHEM IARC
- ▶  Agents Classified by the IARC Monographs, Volumes 1-102
- ▶  Japan's Summary of Initial Risk Assessments
- ▶  NLM TOXNET HSDB URL

Chronic Toxicity

Show Data Hide Data

- ▶  CPDB Report on Carcinogenicity Potency URL (Univ. Cal., Berkeley)
- ▶  DSSTox NTP BSI Chronic / Cancer Study Index
- ▶  DSSTox NTP BSI URL
- ▶  EPA IRIS (Integrated Risk Information System)
- ▶  INCHEM Environmental Health Criteria Monographs
- ▶  INCHEM IARC
- ▶  Agents Classified by the IARC Monographs, Volumes 1-102
- ▶  Japan's Summary of Initial Risk Assessments
- ▶  NTP Long Term Toxicology / Carcinogenicity Study Abstracts and Reports
- ▶  NLM TOXNET HSDB URL

Carcinogenicity

Show Data Hide Data

- ▶  Project Results for California Teachers Study (CTS)
- ▶  CheLIST combination of files from EU Research lists
- ▶  CPDB Report on Carcinogenicity Potency URL (Univ. Cal., Berkeley)
- ▶  DSSTox Cancer Potency Database Summary
- ▶  DSSTox Cancer Potency Database URL
- ▶  DSSTox NTP BSI Chronic / Cancer Study Index
- ▶  DSSTox NTP BSI URL
- ▶  DSSTox IRIS Study Summaries
- ▶  DSSTox IRIS URLs
- ▶  EPA IRIS (Integrated Risk Information System)
- ▶  EPA mid-Atlantic Region Human Health Risk-Based Concentrations
- ▶  EPA Mid-Atlantic Region Protection of Groundwater (screening levels)
- ▶  EPA Southwest region Region Human Health Risk-Based Concentrations
- ▶  Health Canada Priority Substance Lists (2006) (Carcinogenicity)
- ▶  Agents Classified by the IARC Monographs, Volumes 1-111
- ▶  INCHEM Environmental Health Criteria Monographs
- ▶  INCHEM IARC
- ▶  Agents Classified by the IARC Monographs, Volumes 1-102
- ▶  Japan's Summary of Initial Risk Assessments
- ▶  NTP Long Term Toxicology / Carcinogenicity Study Abstracts and Reports
- ▶  OSHA Chemical Sampling Information
- ▶  Risk Assessment Information System Carcinogenicity Metadata
- ▶  Chemical and Physical properties from Risk Assessment Information System (RAIS)
- ▶  NLM TOXNET HSDB URL
- ▶  NLM TOXNET HSDB Carcinogenicity
- ▶  NLM TOXNET CCRIS URL
- ▶  NLM TOXNET CCRIS Data CSTU - CARCINOGENICITY STUDIES

Genotoxicity

Developmental Toxicity

Reproductive Toxicity

Biomonitoring

Occurrence

HEALTH HAZARDS

	Hazard class	Classification	Symbol	Signal word	Hazard statement	Rationale for the classification
1	Acute toxicity (Oral)	Category 5	–	Warning	May be harmful if swallowed	Rat LD50 value: 3500mg/kg (MOE Risk Assessment vol.4, 2005, EHC 111, 1991), 3800mg/kg (EHC 111, 1999, ACGIH 7th, 2001, DFGOT vol.2, 1991), 10800mg/kg (EHC 111, 1991, DFGOT vol.2, 1991), >5000mg/kg (EHC 111, 1991) and >6400mg/kg (PATTY 4th, 1994). Calculated based on the data above. Since the calculated values was 3723.1mg/kg, it was classified to category 5.
1	Acute toxicity (Dermal)	Not classified	–	–	–	Based on rabbit LD50 value: >7900mg/kg (MOE Risk Assessment the 4th volume, 2005, EHC 111, 1991, DFGOT vol.2, 1991), and >10000mg/kg (DFGOT vol.2, 1991), it was set as the outside of Category.
1	Acute toxicity (Inhalation: Gases)	Not applicable	–	–	–	Solid (GHS definition)
1	Acute toxicity (Inhalation: Vapours)	Classification not possible	–	–	–	No data available
1	Acute toxicity (Inhalation: Dusts and mists)	Classification not possible	–	–	–	No data available
2	Skin corrosion/irritation	Not classified	–	–	–	From description that irritation was not admitted in the test applied to the skin of the rat for 4 hours on DFGOT (2 vol. 1991) and ACGIH (7th, 2001), it was carried out the outside of Category.
3	Serious eye damage/eye irritation	Category 2B	–	Warning	Causes eye irritation	We classified it as Category 2B based on the description that a slight conjunctival reddening was acknowledged and it disappeared within 7 days in the test applied to the eyes of the rabbits (DFGOT(vol.2,1991)).
4	Respiratory sensitization	Classification not possible	–	–	–	No data
4	Skin sensitization	Classification not possible	–	–	–	ACGIH (7th, 2001) and HSDB (2006) had description of the case report of allergic contact dermatitis, however, both of which were considered to be the same description of one case and did not have the report of two or more cases which is a judging standard of skin sensitization, and we thought the data was insufficient, therefore we presupposed that we could not classify it.
5	Germ cell mutagenicity	Classification not possible	–	–	–	Classification not possible due to lack of data
6	Carcinogenicity	Not classified	–	–	–	Since it was classified into A4 in ACGIH (ACGIH 7th, 2001), it was considered as the outside of Category.
7	Reproductive toxicity	Not classified	–	–	–	It was considered as out of Category based on the description that clear reproductive toxicity was not observed at the dose as which general toxicity is observed in parent animals in the test administered orally before mating till the term pregnancy using rat (MOE Risk Assessment 4th volume (2005), ACGIH (7th, 2001), and EHC 111 (1991)).
8	Specific target organ toxicity – Single exposure	Classification not possible	–	–	–	Insufficient data available.
9	Specific target organ toxicity – Repeated exposure	Not classified	–	–	–	We classified it into Out Of Category based on the description that in the oral study using the rat, the serious toxic effect was not observed with the dose which exceeds the guidance value range of Category 2 (MOE Risk Assessment The 4th volume (2005), EHC 111 (1991), DFGOT (vol.2, 1991) and ACGIH (7th, 2001)).
10	Aspiration hazard	Classification not possible	–	–	–	No data available

ENVIRONMENTAL HAZARDS

	Hazard class	Classification	Symbol	Signal word	Hazard statement	Rationale for the classification
11	Hazardous to the aquatic environment (Acute)	Category 1	Environment	Warning	Very toxic to aquatic life	It was classified into Category 1 from 96-hour LC50=0.18-0.32mg/L of Crustacea (Mysid shrimp) (EHC111, 1991).
11	Hazardous to the aquatic environment (Long-term)	Category 1	Environment	Warning	Very toxic to aquatic life with long lasting effects	Classified into Category 1, since acute toxicity is Category 1, and supposedly bioaccumulative (log Kow=4.59(PHYSPPROP Database, 2005)), though rapidly degrading (BOD: 90% [existing chemical substances safety inspections data]).

Greenscreen scores from NITE*

108-95-2.json ×

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        "symbol": " - "
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        "hazard_id": 1.0,
        "hazard_name": "Acute toxicity Dermal",
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        "rationale": "Based on the testing data of rat LD50 (dermal r",
        "signal_word": "Danger",
        "symbol": "Skull and crossbones"
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  },
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      "AT": 4,
      "B": 0,
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      "CA": 0,
      "D": 4,
      "E": 0,
      "F": 2,
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      "P": 0,
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      "Rx": 2,
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      "SnS": 2
    }
  }
]
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*Wehage, K., Chenhansa, P. and Schoenung, J. M. (2017), An open framework for automated chemical hazard assessment based on GreenScreen for Safer Chemicals: A proof of concept. Integr Environ Assess Manag, 13: 167–176



Triphenyl phosphate

CAS: 115-86-6

Stronger effect /
evidence



Weaker effect /
evidence

How can this chemical affect my health?

■ Acute (Short Term) Effects [Data sources](#)



Toxic to Humans & Animals – Can be fatal on contact, ingestion or inhalation for humans and other mammals.



Irritates the Eyes – Can cause irritation or serious damage to the eye.

■ Chronic (Long Term) Effects [Data sources](#)



Endocrine Disruption – Can interfere with hormone communication between cells which controls metabolism, development, growth, reproduction and behavior (the endocrine system).



Brain/Nervous System Harm – Can cause damage to the nervous system including the brain.

Inherent Hazards [Data sources](#)



Restricted List – This chemical is on a list from an authoritative body recommending that its use be avoided.

How does this chemical impact the environment?



Immediate Harm to Aquatic Ecosystems – A single exposure may result in severe biological harm or death to fish or other aquatic organisms.



Long-Term Harm to Aquatic Ecosystems – Long term exposure may result in irreversible harm to fish or other aquatic organisms.



Bioaccumulative – Accumulates in organisms, concentrating as it moves up the food chain.



Persistent – Does not break down readily from natural processes.

Data sources:

Direct Hazard » Toxic to Humans & Animals

These sources refer directly to this chemical:

- Acute toxicity (oral) - Category 5

Japan GHS Classifications

Government of Japan

- 6.1D (oral) - Acutely toxic

New Zealand HSNO Chemical Classifications

New Zealand Environmental Protection Authority (NZ EPA)

Direct Hazard » Irritates the Eyes

These sources refer directly to this chemical:

- Serious eye damage / eye irritation - Category 2B

Japan GHS Classifications

Government of Japan

- 6.4A - Irritating to the eye (Cat. 2A)

New Zealand HSNO Chemical Classifications

New Zealand Environmental Protection Authority (NZ EPA)

GHS Scores from ChemHAT

Priority	Source	Acute Tox Score			
		VH	H	M	L
1	EU_H	H300	H301	H302	
2	EU_R	R28	R25	R22	
3	New Zealand	6.1A, 6.1B	6.1C	6.1D	6.1E
4	Japan (NITE)	Cat 1, Cat 2	Cat 3	Cat 4	Cat 5
5	Australia	H300	H301	H302	
6	Korea	H300	H301	H302	
7	Malaysia	H300	H301	H302	
8	WHMIS-SIMDUT	D1A	D1B		

Priority	Source	Eye Irritation Score			
		VH	H	M	L
1	EU_H	H318	H319	H320	
2	EU_R	R41	R36		
3	New Zealand	Cat 1	Cat 2A		
4	Japan (NITE)	Cat 1	Cat 2A	Cat 2B	
5	Australia	H318	H319	H320	
6	Korea	H318	H319	H320	
7	Malaysia	H318	H319	H320	

Data sources:

Direct Hazard » Toxic to Humans & Animals

These sources refer directly to this chemical:

- Acute toxicity (oral) - Category 5
Japan GHS Classifications
Government of Japan
- 6.1D (oral) - Acutely toxic
New Zealand HSNO Chemical Classification
New Zealand Environmental Protection Authority (EPA)

Direct Hazard » Irritates the Eyes

These sources refer directly to this chemical:

- Serious eye damage / eye irritation - Category 2B
Japan GHS Classifications
Government of Japan
- 6.4A - Irritating to the eye (Cat. 2A)
New Zealand HSNO Chemical Classification
New Zealand Environmental Protection Authority (EPA)

L

M

M

H

M

H

Sources of acute toxicity data in ChemHat

Source	# chemicals
EU H Score	1631
EU R Score	1498
New Zealand	1402
Japan	877
Australia	1626
Korea	567
Malaysia	138
WHMIS-SIMDUT	378
All sources	2873

Bis(pentabromophenyl) ether



EC number: 214-604-9 | CAS number: 1163-19-5

- General information**
- Classification & Labelling & PBT assessment**
- Manufacture, use & exposure**
- Physical & Chemical properties**
- Environmental fate & pathways**
- Ecotoxicological information**
- Toxicological information**

- Toxicological Summary
- ▶ **Toxicokinetics, metabolism and distribution**
- ▶ **Acute Toxicity**
 - Endpoint summary
 - Acute Toxicity: oral
 - Acute Toxicity: inhalation
 - Acute Toxicity: dermal
 - Acute Toxicity: other routes
- ▶ **Irritation / corrosion**
- ▶ **Sensitisation**
- ▶ **Repeated dose toxicity**
- ▶ **Genetic toxicity**
 - Carcinogenicity
- ▶ **Toxicity to reproduction**
 - Specific investigations
 - Exposure related observations in humans
 - Toxic effects on livestock and pets
 - Additional toxicological data

Acute Toxicity: oral

Administrative data | Data source | Materials and methods | Results and discussion | Applicant's summary and conclusion

Administrative data

Endpoint: acute toxicity: oral

Type of information: experimental study

Adequacy of study: key study

Reliability: 2 (reliable with restrictions)

Data source

Reference

+ Reference 1

+ Reference 2

Effect levels

Sex: female

Dose descriptor: LD50

Effect level: > 2 000 mg/kg bw

Based on: test mat.

Applicant's summary and conclusion

Interpretation of results: practically nontoxic

REACH Field Mapping

GHS Category	Link in REACH dossier
Acute Toxicity	Acute Toxicity: oral / inhalation / dermal
Carcinogenicity	Carcinogenicity
Genotoxicity / Mutagenicity	Genetic toxicity: in vitro / in vivo
Endocrine Disruption	N/A
Reproductive	Toxicity to reproduction
Developmental	Developmental toxicity / teratogenicity
Neurological	Neurotoxicity
Repeated Dose	Repeated dose toxicity: oral / inhalation / dermal
Skin Sensitization	Skin sensitisation
Eye Irritation	Eye irritation
Dermal Irritation	Skin irritation / corrosion
Acute aquatic	Short-term toxicity to fish
Chronic aquatic	Long-term toxicity to fish
Persistence	Biodegradation in water: screening tests
Bioaccumulation	Bioaccumulation: aquatic / sediment

Steps for obtaining REACH dossier data

- Download list of chemicals (get dossier numbers)
- Download records for given endpoint
- Parse html files (using Java code) to JSON files
- Convert JSON files to flat text file
- Omit records with wrong test type, poor reliability, QSAR, estimated values, ambiguous results
- Determine best CAS number from available fields
- Omit “bad” chemicals in terms of QSAR (e.g. polymers, salts, unspecified structure) based on SciFinder record for given CAS number
- Omit duplicate records (need 80% agreement for binary endpoint)

The Global Portal to Information on Chemical Substances



eChemPortal

eChemPortal

- Home
- Substance Search
- Property Search**
- GHS Search
- What's new?
- General Information
- Participating Databases
- Roles & Responsibilities
- Linking to eChemPortal
- Schedules of Assessments
- Structure Search
- GHS Classifications
- Useful links
- FAQ
- How to search for information
- Contact us
- Disclaimer

Skin sensitisation

Define the search criteria for the Query Block.

Cancel Save

Study result type:

experimental result

Reliability:

1 (reliable without restriction)|2 (reliable with restrictions)

Reference, Year:

=

Type of method:

Type of study:

Guinea pig maximisation test

Test guideline, Qualifier:

Test guideline, Guideline:

OECD Guideline 406 (Skin Sensitisation)

GLP compliance:

Species:

guinea pig

Strain:

Interpretation of results:

not sensitising|sensitising

Cancel Save

Tested substance is important!

From REACH dossier for tetradec-1-ene

Record #	Name of test material	Substance type
15664_016	SHOP C68 Internal Olefin	Alkenes, C6-8
2040_016	SHOP C68 Internal Olefin	Alkenes, C6-8
15664_017	NEODENE-8	C8 alpha olefin
2040_017	NEODENE-8	C8 alpha olefin
15664_018	SHOP C134 Internal Olefin	Alkenes, C11/C13/C14
2040_018	SHOP C134 Internal Olefin	Alkenes, C11/C13/C14
15664_019	Internal Olefin 114 LP11	Alkenes, C11-15
2040_019	Internal Olefin 114 LP11	Alkenes, C11-15
15664_027	C20-C24 Alkenes, Branched and Linear	Alkenes, C20-24
2040_027	C20-C24 Alkenes, Branched and Linear	Alkenes, C20-24
15664_028	ENORDET O241	
2040_028	ENORDET O241	

Skin sensitisation

Currently viewing:

002 Key | Experimental result

Administrative data

Data source

Materials and methods

Results and discussion

Applicant's summary and conclusion

Qualifier:

equivalent or similar to

Guideline:

OECD Guideline 406 (Skin Sensitisation)

GLP compliance:

yes

Type of study:

guinea pig maximisation test

Justification for non-LLNA method:

The study was conducted in accordance with OECD and EU test guidelines applicable at the time of undertaking.

Test material

Reference

Name:

Unnamed

Type:

Constituent

Details on test material:

- Name of test material (as cited in study report): SHOP C68 Internal Olefin

- Substance type: Alkenes, C6-8

- Physical state: Liquid (clear, colourless)

- Lot/batch No.: 168082

- Storage condition of test material: Cool conditions (not exceeding 15 degrees C), under nitrogen, protected from light, in the original container.

All tests are “not sensitizing” so we can still learn from it qualitatively

[illegible]

Questions???

The views expressed in this presentation are those of the author and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency