

# Safety data sheet

acc. to Safe Work Australia - Code of Practice



## Acetylacetone $\geq 98\%$ , for synthesis

article number: **6716**  
Version: **GHS 3.0 en**  
Replaces version of: 2021-06-11  
Version: (GHS 2)

date of compilation: 2016-11-08  
Revision: 2024-03-02

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifier

Identification of the substance	<b>Acetylacetone <math>\geq 98\%</math>, for synthesis</b>
Article number	6716
CAS number	123-54-6
Alternative name(s)	Pentane-2,4-dione

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feeding-stuffs.

### 1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:** +49 (0) 721 - 56 06 0  
**Telefax:** +49 (0) 721 - 56 06 149  
**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)  
**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 Westmead, NSW	131126	

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	3	Flam. Liq. 3	H226
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302
3.1D	Acute toxicity (dermal)	3	Acute Tox. 3	H311

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.1I	Acute toxicity (inhal.)	3	Acute Tox. 3	H331

For full text of abbreviations: see SECTION 16

### The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

## 2.2 Label elements

### Labelling

#### Signal word

**Danger**

#### Pictograms

GHS02, GHS06



#### Hazard statements

H226 Flammable liquid and vapour  
H302 Harmful if swallowed  
H311+H331 Toxic in contact with skin or if inhaled

#### Precautionary statements

##### Precautionary statements - prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
P280 Wear protective gloves/protective clothing

##### Precautionary statements - response

P302+P352 IF ON SKIN: Wash with plenty of soap and water  
P370+P378 In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction

##### Precautionary statements - storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed  
P403+P235 Store in a well-ventilated place. Keep cool

## 2.3 Other hazards

### Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

### Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Acetylacetone
Molecular formula	$C_5H_8O_2$
Molar mass	100.1 $g/mol$
CAS No	123-54-6

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off immediately all contaminated clothing.

#### Following inhalation

Call a physician immediately. If breathing is irregular or stopped, administer artificial respiration.

#### Following skin contact

After contact with skin, wash immediately with plenty of water.

#### Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

### 4.2 Most important symptoms and effects, both acute and delayed

Irritant effects, Nausea, Vomiting, Cough, Headache, Vertigo, Dyspnoea

### 4.3 Indication of any immediate medical attention and special treatment needed

none

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!  
water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

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### 5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

#### Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures



#### For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

### 6.3 Methods and material for containment and cleaning up

#### Advice on how to contain a spill

Covering of drains.

#### Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

### 6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Provision of sufficient ventilation. Use extractor hood (laboratory). Handle and open container with care. Clear contaminated areas thoroughly.

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### Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

#### Advice on general occupational hygiene

Thorough skin-cleansing after handling the product. When using do not smoke.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice:

Store locked up. Ground/bond container and receiving equipment.

#### Ventilation requirements

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted. Use local and general ventilation.

#### Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

#### Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

#### Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	84 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	12 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

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### Environmental values

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0.2 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0.02 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	1.32 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	1.909 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0.191 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0.193 mg/kg	terrestrial organisms	soil	short-term (single instance)

## 8.2 Exposure controls

### Individual protection measures (personal protective equipment)

#### Eye/face protection



Use safety goggle with side protection.

#### Skin protection



#### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

#### • type of material

Butyl caoutchouc (butyl rubber)

#### • material thickness

0,7mm

#### • breakthrough times of the glove material

>480 minutes (permeation: level 6)

#### • Splash protection - Protective gloves

• type of material: NBR (Nitrile rubber)

• material thickness: 0,4 mm

• breakthrough times of the glove material: >30 minutes (permeation: level 2)

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### • other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

### Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of  $> 65\text{ }^{\circ}\text{C}$ , colour code: Brown).

### Environmental exposure controls

Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless - light yellow
Odour	disagreeable
Melting point/freezing point	$-47.5 - -17.6\text{ }^{\circ}\text{C}$ at 1,013 hPa (ECHA)
Boiling point or initial boiling point and boiling range	$139.5\text{ }^{\circ}\text{C}$ at 1,013 hPa (ECHA)
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	2.4 vol% (LEL) - 11.4 vol% (UEL)
Flash point	$35\text{ }^{\circ}\text{C}$ at 95.6 kPa (ECHA)
Auto-ignition temperature	$390\text{ }^{\circ}\text{C}$ at 960.6 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	6 (in aqueous solution: 200 g/l, $20\text{ }^{\circ}\text{C}$ )
Kinematic viscosity	$0.7856\text{ mm}^2/\text{s}$ at $20\text{ }^{\circ}\text{C}$
Dynamic viscosity	$0.762\text{ mPa s}$ at $20\text{ }^{\circ}\text{C}$ $0.625\text{ mPa s}$ at $40\text{ }^{\circ}\text{C}$
<u>Solubility(ies)</u>	
Water solubility	$\leq 155.2\text{ g/l}$ at $20\text{ }^{\circ}\text{C}$ (ECHA)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	0.68 (pH value: $-7$ , $40\text{ }^{\circ}\text{C}$ ) (ECHA)
<u>Vapour pressure</u>	
	$7.9\text{ hPa}$ at $20\text{ }^{\circ}\text{C}$ $40.4\text{ hPa}$ at $50\text{ }^{\circ}\text{C}$
<u>Density and/or relative density</u>	
Density	$0.97\text{ g/cm}^3$ at $20\text{ }^{\circ}\text{C}$ (ECHA)

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Relative vapour density 3.5 (air = 1)

Particle characteristics not relevant (liquid)

### Other safety parameters

Oxidising properties none

## 9.2 Other information

Information with regard to physical hazard classes: There is no additional information.

Other safety characteristics:

Surface tension 72 mN/m (20 °C) (ECHA)

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

It's a reactive substance. Risk of ignition.

#### **If heated**

Risk of ignition. Vapours may form explosive mixtures with air.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

**Violent reaction with:** Aldehydes, Alkali metals, Amines, Bases, Halogenated hydrocarbons, Oxidisers, Acids

### 10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

### 10.5 Incompatible materials

different plastics, copper, Steel, zinc

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5. Peroxides.

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### **Classification acc. to GHS**

#### **Acute toxicity**

Harmful if swallowed. Toxic in contact with skin. Toxic if inhaled.



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Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
inhalation: vapour	LC50	5.1 mg/l/4h	rat		ECHA
oral	LD50	570 mg/kg	rat		ECHA
dermal	LD50	790 mg/kg	rabbit		ECHA

### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

### Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

### Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

### Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

### Carcinogenicity

Shall not be classified as carcinogenic.

### Reproductive toxicity

Shall not be classified as a reproductive toxicant.

### Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

### Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

### Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

### Symptoms related to the physical, chemical and toxicological characteristics

#### • If swallowed

vomiting, nausea

#### • If in eyes

slightly irritant but not relevant for classification

#### • If inhaled

vertigo, cough, headache, Dyspnoea

#### • If on skin

Frequently or prolonged contact with skin may cause dermal irritation

#### • Other information

Other adverse effects: Liver and kidney damage

## 11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

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## SECTION 12: Ecological information

### 12.1 Toxicity

Harmful to aquatic life.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	104 mg/l	fish	ECHA	96 h
EC50	25.9 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	83.22 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	107.6 mg/l	microorganisms	ECHA	3 h

### 12.2 Persistence and degradability

Theoretical Oxygen Demand: 1.918 mg/mg  
Theoretical Carbon Dioxide: 2.198 mg/mg

#### Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
biotic/abiotic	79 – 88 %	28 d
carbon dioxide generation	83 – 100 %	28 d

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	0.68 (pH value: ~7, 40 °C) (ECHA)
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### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

### 12.7 Other adverse effects

Data are not available.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

#### Sewage disposal-relevant information

Do not empty into drains.

#### Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

#### Relevant provisions relating to waste(Basel Convention)

#### Properties of waste which render it hazardous

H3 Flammable liquids

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

## SECTION 14: Transport information

### 14.1 UN number

UN RTDG	UN 2310
IMDG-Code	UN 2310
ICAO-TI	UN 2310

### 14.2 UN proper shipping name

UN RTDG	PENTANE-2,4-DIONE
IMDG-Code	PENTANE-2,4-DIONE
ICAO-TI	Pentane-2,4-dione

### 14.3 Transport hazard class(es)

UN RTDG	3 (6.1)
IMDG-Code	3 (6.1)
ICAO-TI	3 (6.1)

### 14.4 Packing group

UN RTDG	III
IMDG-Code	III
ICAO-TI	III

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**14.5 Environmental hazards** non-environmentally hazardous acc. to the dangerous goods regulations

**14.6 Special precautions for user**  
There is no additional information.

**14.7 Transport in bulk according to IMO instruments**  
The cargo is not intended to be carried in bulk.

### 14.8 Information for each of the UN Model Regulations

#### Transport information National regulations Additional information (UN RTDG)

**UN number** 2310

**Class** 3

**Subsidiary risk(s)** 6.1

**Packing group** III

**Danger label(s)** 3+6.1



**Special provisions (SP)** -  
UN RTDG

**Excepted quantities (EQ)** E1  
UN RTDG

**Limited quantities (LQ)** 5 L  
UN RTDG

**Emergency Action Code** 2Y

#### International Maritime Dangerous Goods Code (IMDG) - Additional information

**Proper shipping name** PENTANE-2,4-DIONE

**Particulars in the shipper's declaration** UN2310, PENTANE-2,4-DIONE, 3 (6.1), III, 35°C c.c.

**Marine pollutant** -

**Danger label(s)** 3+6.1



**Special provisions (SP)** -

**Excepted quantities (EQ)** E1

**Limited quantities (LQ)** 5 L

**EmS** F-E, S-D

**Stowage category** A

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### International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Proper shipping name	Pentane-2,4-dione
Particulars in the shipper's declaration	UN2310, Pentane-2,4-dione, 3 (6.1), III
Danger label(s)	3+6.1
	
Excepted quantities (EQ)	E1
Limited quantities (LQ)	2 L

## SECTION 15: Regulatory information

### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

There is no additional information.

#### National regulations(Australia)

##### Australian Inventory of Chemical Substances(AICS)

Substance is listed.

#### Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

#### National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

#### Legend

AIIC	Australian Inventory of Industrial Chemicals
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China

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### Legend

INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

## 15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

## SECTION 16: Other information

### Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$ .	yes
14.8		Emergency Action Code: 2Y	yes
15.1		Other information: Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.	yes
15.1		National inventories: change in the listing (table)	yes

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
ErC50	$\equiv$ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization

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Abbr.	Descriptions of used abbreviations
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
UEL	Upper explosion limit (UEL)
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative

### Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

### List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H331	Toxic if inhaled.

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.