

# Safety data sheet

Safe Work Australia - Code of Practice



## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: **2902**  
Version: **GHS 1.0 en**

date of compilation: 2019-06-17

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

#### 1.1 Product identifier

Identification of the substance	<b>4-Acetylbenzonitrile</b>
Article number	2902
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a)
EC number	215-885-0
CAS number	1443-80-7

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

<b>Identified uses:</b>	laboratory and analytical use laboratory chemical
-------------------------	--

#### 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	

Emergency information service

**Poison Centre Munich: +49/(0)89 19240**

### SECTION 2: Hazards identification

#### 2.1 Classification of the substance or mixture

**Classification acc. to GHS**

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.1O	acute toxicity (oral)	(Acute Tox. 4)	H302
3.1D	acute toxicity (dermal)	(Acute Tox. 5)	H313

# Safety data sheet

Safe Work Australia - Code of Practice



## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### 2.2 Label elements

#### Labelling GHS

##### Signal word

Warning

##### Pictograms

GHS07



##### Hazard statements

H302 Harmful if swallowed  
H313 May be harmful in contact with skin

##### Precautionary statements

###### Precautionary statements - prevention

P264 Wash thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.

###### Precautionary statements - response

P301+P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.  
P312 Call a POISON CENTER or doctor/physician if you feel unwell.  
P330 Rinse mouth.

###### Precautionary statements - disposal

P501 Dispose of contents/container to industrial combustion plant.

##### Labelling of packages where the contents do not exceed 125 ml

Signal word: **Warning**

Symbol(s)



H313 May be harmful in contact with skin.  
P312 Call a POISON CENTER or doctor/physician if you feel unwell.

### 2.3 Other hazards

There is no additional information.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	4-Acetylbenzonitrile
EC number	215-885-0
CAS number	1443-80-7
Molecular formula	C <sub>9</sub> H <sub>7</sub> NO
Molar mass	145.2 g/mol

## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### SECTION 4: First aid measures

#### 4.1 Description of first aid measures



##### General notes

Take off contaminated clothing.

##### Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

##### Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

##### 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). Let water be drunken in little sips (dilution effect). Call a doctor.

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

Nausea, Vomiting, Gastrointestinal complaints

#### 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 fire-fighting measures to the fire surroundings  
water spray, foam, dry extinguishing powder, carbon dioxide (CO<sub>2</sub>)

##### Unsuitable extinguishing media

water jet

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

Combustible.

##### Hazardous combustion products

In case of fire may be liberated: nitrogen oxides (NO<sub>x</sub>), carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>)

#### 5.3 Advice for firefighters

Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### 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 dust.

#### 6.2 Environmental precautions

Keep away from drains, surface and ground water.

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

##### Advices on how to contain a spill

Covering of drains.

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

Take up mechanically. Control of dust.

##### 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.

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

Removal of dust deposits.

##### Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

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

Store in a dry place.

##### Incompatible substances or mixtures

Observe hints for combined storage.

##### Consideration of other advice

##### • Ventilation requirements

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.

## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### SECTION 8: Exposure controls/personal protection

#### 8.1 Control parameters

##### National limit values

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

Data are not available.

#### 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. 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.

- **type of material**

NBR (Nitrile rubber)

- **material thickness**

>0,11 mm

- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

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

##### Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P2 (filters at least 94 % of airborne particles, colour code: White).

##### Environmental exposure controls

Keep away from drains, surface and ground water.

## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

##### Appearance

Physical state	solid (solid matter)
Colour	light yellow - beige
Odour	characteristic
Odour threshold	No data available

##### Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	≥57 – ≤58 °C
Initial boiling point and boiling range	264.3 °C
Flash point	131.2 °C
Evaporation rate	no data available
Flammability (solid, gas)	These information are not available

##### Explosive limits

• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	these information are not available
Vapour pressure	0.856 Pa at 25 °C
Density	1.555 g/cm <sup>3</sup> at 25 °C
Vapour density	This information is not available.
Relative density	Information on this property is not available.

##### Solubility(ies)

Water solubility	3,930 mg/l at 25 °C
------------------	---------------------

##### Partition coefficient

n-octanol/water (log KOW)	1.531 (pH value: 5.5, 25 °C) (ECHA)
Soil organic carbon/water (log KOC)	2.214 (ECHA)
Auto-ignition temperature	Information on this property is not available.
Decomposition temperature	no data available
Viscosity	not relevant (solid matter)
Explosive properties	Shall not be classified as explosive
Oxidising properties	none

#### 9.2 Other information

There is no additional information.	
Surface tension	0.045 N/m

## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### SECTION 10: Stability and reactivity

#### 10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

#### 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: Strong oxidiser

#### 10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

#### 10.5 Incompatible materials

There is no additional information.

#### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

### SECTION 11: Toxicological information

#### 11.1 Information on toxicological effects

##### Acute toxicity

Exposure route	Endpoint	Value	Species	Source
oral	LD50	>800 mg/kg	rat	ECHA
dermal	LD50	>2,000 mg/kg	rat	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.

##### Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor 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

## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

nausea, vomiting, gastrointestinal complaints

• **If in eyes**

data are not available

• **If inhaled**

data are not available

• **If on skin**

data are not available

**Other information**

None

## SECTION 12: Ecological information

### 12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

**Aquatic toxicity (acute)**

Endpoint	Value	Species	Source	Exposure time
LC50	162 mg/l	Pimephales promelas	ECHA	96 h
EC50	21.4 mg/l	daphnia magna	ECHA	48 h
ErC50	129.3 mg/l	Grünalge	ECHA	72 h

### 12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 2.48 mg/mg

Theoretical Oxygen Demand: 2.094 mg/mg

Theoretical Carbon Dioxide: 2.729 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)

1.531 (pH value: 5.5, 25 °C)

### 12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient

2.214

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Other adverse effects

Data are not available.



## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### 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.

#### Sewage disposal-relevant information

Do not empty into drains.

#### 13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

#### 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.

### SECTION 14: Transport information

14.1	UN number	(not subject to transport regulations)
14.2	UN proper shipping name	not relevant
14.3	Transport hazard class(es)	not relevant
	Class	-
14.4	Packing group	not relevant not assigned to a packing group
14.5	Environmental hazards	none (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 Annex II of MARPOL and the IBC Code	
	The cargo is not intended to be carried in bulk.	
14.8	Information for each of the UN Model Regulations	
	• <b>Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)</b>	
	Not subject to ADR, RID and ADN.	
	• <b>International Maritime Dangerous Goods Code (IMDG)</b>	
	Not subject to IMDG.	
	• <b>International Civil Aviation Organization (ICAO-IATA/DGR)</b>	
	Not subject to ICAO-IATA.	

## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

### SECTION 15: Regulatory information

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

##### National inventories

Substance is listed in the following national inventories:

Country	National inventories	Status
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
TW	TCSI	substance is listed

##### Legend

ECSI EC Substance Inventory (EINECS, ELINCS, NLP)  
 REACH Reg. REACH registered substances  
 TCSI Taiwan Chemical Substance Inventory

#### 15.2 Chemical Safety Assessment

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

### SECTION 16: Other information

##### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
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
IMDG	International Maritime Dangerous Goods Code
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
vPvB	very Persistent and very Bioaccumulative

# Safety data sheet

Safe Work Australia - Code of Practice



## 4-Acetylbenzonitrile ROTI(R)Calipure Melting point standard

article number: 2902

---

### Key literature references and sources for data

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

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

Code	Text
H302	harmful if swallowed
H313	may be harmful in contact with skin

### Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.