

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt ≥98 %, for ion-pair chromatography

article number: **KK56**  
Version: **2.0 en**  
Replaces version of: 2020-02-19  
Version: (1)

date of compilation: 2020-02-19  
Revision: 2022-08-09

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

### 1.1 Product identifier

Identification of the substance	<b>Pentane-1-sulphonic acid sodium salt</b> ≥98 %, for ion-pair chromatography
Article number	KK56
EC number	245-208-4
CAS number	22767-49-3
Alternative name(s)	Sodium-1-pentane sulphonate

### 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).

### 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
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification acc. to GHS

This substance does not meet the criteria for classification.

### 2.2 Label elements

#### Labelling

not required

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt $\geq 98\%$ , for ion-pair chromatography

article number: **KK56**

### 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.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Pentane-1-sulphonic acid sodium salt
Molecular formula	$C_5H_{11}NaO_3S$
Molar mass	174,2 $g/mol$
CAS No	22767-49-3
EC No	245-208-4

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

No special measures are necessary.

#### 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.

#### 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. Call a doctor if you feel unwell.

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

Symptoms and effects are not known to date.

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

none

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



Pentane-1-sulphonic acid sodium salt  $\geq 98\%$ , for ion-pair chromatography

article number: **KK56**

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings  
water, foam, dry extinguishing powder, ABC-powder

#### 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: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Sulphur oxides (SO<sub>x</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.

## SECTION 6: Accidental release measures

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



#### For non-emergency personnel

Control of dust.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water.

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

#### Advice on how to contain a spill

Covering of drains. Take up mechanically.

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

Take up mechanically.

#### Other information relating to spills and releases

Place in appropriate containers for disposal.

### 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.

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



Pentane-1-sulphonic acid sodium salt  $\geq 98\%$ , for ion-pair chromatography

article number: **KK56**

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

No special measures are necessary.

#### Advice on general occupational hygiene

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.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

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

Country	Name of agent	CAS No	Identifier	TWA [mg/m <sup>3</sup> ]	STEL [mg/m <sup>3</sup> ]	Ceiling-C [mg/m <sup>3</sup> ]	Notation	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

#### Notation

Ceiling-C Ceiling value is a limit value above which exposure should not occur

i Inhalable fraction

r Respirable fraction

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)

#### Eye/face protection



Use safety goggle with side protection.

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt $\geq 98\%$ , for ion-pair chromatography

article number: **KK56**

### Skin protection



- **hand protection**

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

- **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). P1 (filters at least 80 % of airborne particles, colour code: White).

### 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	solid
Form	powder
Colour	white
Odour	odourless
Melting point/freezing point	300 °C
Boiling point or initial boiling point and boiling range	not determined
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	not applicable
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	5,5 – 7,5 (in aqueous solution: 100 g/l, 20 °C)

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt ≥98 %, for ion-pair chromatography

article number: **KK56**

Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	not determined
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	this information is not available
Vapour pressure	not determined
<u>Density and/or relative density</u>	
Density	not determined
Relative vapour density	information on this property is not available
Particle characteristics	No data available.
<u>Other safety parameters</u>	
Oxidising properties	none
<b>9.2 Other information</b>	
Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	There is no additional information.

## 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.

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



**Pentane-1-sulphonic acid sodium salt ≥98 %, for ion-pair chromatography**

article number: **KK56**

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

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

This substance does not meet the criteria for classification.

#### **Acute toxicity**

Shall not be classified as acutely toxic.

#### **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**

Data are not available.

##### **• If in eyes**

Data are not available.

##### **• If inhaled**

Data are not available.

##### **• If on skin**

Data are not available.

##### **• Other information**

Health effects are not known.

### 11.2 Endocrine disrupting properties

Not listed.

### 11.3 Information on other hazards

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt $\geq 98\%$ , for ion-pair chromatography

article number: **KK56**

There is no additional information.

### SECTION 12: Ecological information

#### 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

#### Biodegradation

Data are not available.

#### 12.2 Process of degradability

Theoretical Oxygen Demand: 1,424 mg/mg  
Theoretical Carbon Dioxide: 1,263 mg/mg

#### 12.3 Bioaccumulative potential

Data are not available.

#### 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

Not listed.

#### 12.7 Other adverse effects

Data are not available.

### SECTION 13: Disposal considerations

#### 13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

#### 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. Waste catalogue ordinance (Germany).

#### 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.



# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt ≥98 %, for ion-pair chromatography

article number: **KK56**

### SECTION 14: Transport information

- 14.1 UN number or ID number** not subject to transport regulations
- 14.2 UN proper shipping name** not assigned
- 14.3 Transport hazard class(es)** none
- 14.4 Packing group** not assigned
- 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 Maritime 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 of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information**

Not subject to ADR, RID and ADN.

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

Not subject to IMDG.

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

Not subject to ICAO-IATA.

### SECTION 15: Regulatory information

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

##### **Relevant provisions of the European Union (EU)**

###### **Seveso Directive**

2012/18/EU (Seveso III)			
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
	not assigned		

###### **Deco-Paint Directive**

VOC content	0 %
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###### **Industrial Emissions Directive (IED)**

VOC content	0 %
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##### **Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)**

not listed

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt ≥98 %, for ion-pair chromatography

article number: **KK56**

### Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

### Water Framework Directive (WFD)

#### List of pollutants (WFD)

Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
Pentane-1-sulphonic acid sodium salt	Metals and their compounds		a)	

#### Legend

A) Indicative list of the main pollutants

### Regulation on the marketing and use of explosives precursors

not listed

### Regulation on drug precursors

not listed

### Regulation on substances that deplete the ozone layer (ODS)

not listed

### Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

### Regulation on persistent organic pollutants (POP)

not listed

### National regulations(GB)

#### List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

#### Restrictions according to GB REACH, Annex 17

not 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
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

#### Legend

AIIC Australian Inventory of Industrial Chemicals

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt ≥98 %, for ion-pair chromatography

article number: **KK56**

### Legend

DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
NZIoC	New Zealand Inventory of Chemicals
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)

Alignment to regulation:

Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1	Classification according to Regulation (EC) No 1272/2008 (CLP): This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.	Classification acc. to GHS: This substance does not meet the criteria for classification.	yes
2.2	Signal word: not required		yes
2.3	Other hazards: There is no additional information.	Other hazards	yes
2.3		Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.	yes

### 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 relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EH40/2005	EH40/2005 Workplace exposure limits ( <a href="http://www.nationalarchives.gov.uk/doc/open-government-licence/">http://www.nationalarchives.gov.uk/doc/open-government-licence/</a> )
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations

# Safety data sheet Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Pentane-1-sulphonic acid sodium salt $\geq 98$ %, for ion-pair chromatography

article number: **KK56**

Abbr.	Descriptions of used abbreviations
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
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)
STEL	Short-term exposure limit
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

### Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

### Disclaimer

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