

SAFETY DATA SHEET

Version 6.4
Revision Date 08/06/2024
Print Date 08/07/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Sulfonic Acids, C10-21-alkane, Phenylesters

Product Number : 50987
Brand : Sigma-Aldrich
CAS-No. : 91082-17-6

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture**

Not a hazardous substance or mixture.

2.2 GHS Label elements, including precautionary statements

No hazard pictogram, no signal word, no hazard statement(s), no precautionary statement(s) required.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Alkylsulfonic phenyl ester

CAS-No. : 91082-17-6

EC-No. : 293-728-5

No components need to be disclosed according to the applicable regulations.

SECTION 4: First aid measures

4.1 Description of first-aid measures

No data available

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

No data available

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Sulfur oxides

Combustible.

5.3 Advice for firefighters

No data available

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.

6.2 Environmental precautions

No data available

6.3 Methods and materials for containment and cleaning up

No data available

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

No data available

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

No data available

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: liquid, clear
Color: light yellow |
| b) Odor | odorless |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | < -15 °C (< 5 °F) |
| f) Initial boiling point and boiling range | 300 - 400 °C 572 - 752 °F - OECD Test Guideline 103 |
| g) Flash point | 210 - 240 °C (410 - 464 °F) - open cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |

k) Vapor pressure	0.000 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	1.04 - 1.07 g/cm ³ at 20 °C (68 °F) - DIN 51757
Relative density	No data available
n) Water solubility	0.0022 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	log Pow: 8.8 - 11.3 at 40 °C (104 °F) - OECD Test Guideline 117
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

No data available

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - > 15,900 mg/kg

Inhalation: No data available

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LD50 Dermal - Rat - > 1,055 mg/kg
No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

No data available

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish semi-static test LC50 - *Oryzias latipes* - > 100 mg/l - 96 h
(OECD Test Guideline 203)

Toxicity to daphnia static test EC0 - *Daphnia magna* (Water flea) - >= 100 mg/l - 48 h

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and other aquatic
invertebrates

Toxicity to algae static test EC0 - *Desmodesmus subspicatus* (green algae) - ≥ 2
mg/l - 72 h

Toxicity to bacteria Respiration inhibition EC50 - Sludge Treatment - $> 10,000$ mg/l - 3
h
(OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 31 % - Not readily biodegradable.
(OECD Test Guideline 301C)

12.3 Bioaccumulative potential

Bioaccumulation *Cyprinus carpio* (Carp) - 36 d
- 1 mg/l (Sulfonic acids, C10-21-alkane, phenylesters)

Bioconcentration factor (BCF): 7 - 39

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not
conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

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Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : No SARA Hazards

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the

information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

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