SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 9.8
Revision Date 04.11.2024
Print Date 30.03.2025
GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1 Product identifiers

Product name : MSMLS Plate 6 (Lipophilic)

Product Number : MSMLS06
Brand : Sigma
REACH No. : This product is a mixture. REACH Registration Number see section 3.

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

Identified uses : Laboratory chemicals, Manufacture of substances
Uses advised against : For R&D use only. Not for pharmaceutical, household or other uses.

1.3 Details of the supplier of the safety data sheet

Company :

1.4 Emergency telephone

Emergency Phone # : +(44)-870-8200418 (CHEMTREC (GB))
+(353)-19014670 (CHEMTREC Ireland)
001-803-017-9114 (CHEMTREC India)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Acute toxicity, (Category 4)	H302: Harmful if swallowed.
Acute toxicity, (Category 1)	H310: Fatal in contact with skin.
Skin irritation, (Category 2)	H315: Causes skin irritation.
Serious eye damage, (Category 1)	H318: Causes serious eye damage.
Skin sensitization, (Category 1)	H317: May cause an allergic skin reaction.
Germ cell mutagenicity, (Category 2)	H341: Suspected of causing genetic defects.
Carcinogenicity, (Category 2)	H351: Suspected of causing cancer.

Long-term (chronic) aquatic hazard, (Category 2)	H411: Toxic to aquatic life with long lasting effects.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H302	Harmful if swallowed.
H310	Fatal in contact with skin.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H341	Suspected of causing genetic defects.
H351	Suspected of causing cancer.
H411	Toxic to aquatic life with long lasting effects.
Precautionary Statements	
P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P302 + P352 + P310	IF ON SKIN: Wash with plenty of water. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word	Danger
Hazard Statements	
H310	Fatal in contact with skin.
H317	May cause an allergic skin reaction.
H341	Suspected of causing genetic defects.
H351	Suspected of causing cancer.
H318	Causes serious eye damage.
Precautionary Statements	
P264	Wash skin thoroughly after handling.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P302 + P352 + P310	IF ON SKIN: Wash with plenty of water. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes.

	Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:
The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
Toxicological information:
The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Component		Classification	Concentration
3-Hydroxyphenyl acetate			
CAS-No. EC-No. *	102-29-4 203-022-0	Acute Tox. 4; Eye Dam. 1; Skin Sens. 1; H302, H318, H317	>= 1 - < 3 %
1-Methyl-6,7-dihydroxy-1,2,3,4-tetrahydroisoquinoline hydrobromide			
CAS-No. *	59709-57-8	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
3-Hydroxybenzoic acid			
CAS-No. EC-No. *	99-06-9 202-726-5	Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H302, H315, H319, H335	>= 1 - < 10 %
Itaconic acid			
CAS-No. EC-No. *	97-65-4 202-599-6	Eye Dam. 1; H318	>= 1 - < 3 %
2-Methylbutyraldehyde			
CAS-No. EC-No.	96-17-3 202-485-6	Flam. Liq. 2; Eye Irrit. 2; Skin Sens. 1; STOT SE 3; Aquatic Chronic 2; H225,	>= 1 - < 2.5 %

	*	H319, H317, H335, H411	
2',4'-Dihydroxyacetophenone			
CAS-No. EC-No.	89-84-9 201-945-3 *	Eye Irrit. 2; H319	>= 1 - < 10 %
Salicylic acid			
CAS-No. EC-No. Index-No. Registration number	69-72-7 200-712-3 607-732-00-5 01-2119486984-17-XXXX	Acute Tox. 4; Eye Dam. 1; Repr. 2; H302, H318, H361d	>= 1 - < 3 %
Salicylamide			
CAS-No. EC-No.	65-45-2 200-609-3 *	Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H302, H315, H319, H335	>= 1 - < 10 %
3-hydroxyphenylacetic acid			
CAS-No. EC-No.	621-37-4 210-684-4 *	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
suberic acid			
CAS-No. EC-No.	505-48-6 208-010-9 *	Eye Irrit. 2; H319	>= 1 - < 10 %
Citraconic acid			
CAS-No. EC-No.	498-23-7 207-858-7 *	Acute Tox. 4; H302	>= 1 - < 10 %
N-Ethyl-2-(isopropyl)-5-methylcyclohexanecarboxamide			
CAS-No. EC-No.	39711-79-0 254-599-0 *	Acute Tox. 4; Eye Dam. 1; H302, H318	>= 1 - < 3 %
O,O'-Bis(3-aminopropyl)polyethylene glycol			
CAS-No.	34901-14-9 *	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
2-Oxo-hexanedioic acid			
CAS-No.	3184-35-8 *	Skin Irrit. 2; Eye Irrit. 2; H315, H319	>= 1 - < 10 %

Indole-3-acetaldehyde sodium bisulfite			
CAS-No.	20095-27-6 *	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
(S)-(-)-1-phenylethanol			
CAS-No.	1445-91-6 *	Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2; H302, H315, H319	>= 1 - < 10 %
trans-Cinnamaldehyde			
CAS-No.	14371-10-9 *	Skin Irrit. 2; Eye Irrit. 2; Skin Sens. 1; STOT SE 3; H315, H319, H317, H335	>= 1 - < 10 %
pyruvic acid			
CAS-No. EC-No.	127-17-3 204-824-3 *	Skin Corr. 1C; Eye Dam. 1; H314, H318	>= 1 - < 3 %
adipic acid			
CAS-No. EC-No. Index-No.	124-04-9 204-673-3 607-144-00-9 *	Eye Dam. 1; H318	>= 1 - < 3 %
Azelaic acid			
CAS-No. EC-No. Registration number	123-99-9 204-669-1 01-2119557891-28-XXXX	Skin Irrit. 2; Eye Irrit. 2; H315, H319	>= 1 - < 10 %
Vanillin			
CAS-No. EC-No. Registration number	121-33-5 204-465-2 01-2119516040-60-XXXX	Eye Irrit. 2; H319	>= 1 - < 10 %
methyl acetoacetate			
CAS-No. EC-No. Index-No.	105-45-3 203-299-8 607-137-00-0 *	Eye Dam. 1; H318	>= 1 - < 3 %
4-Methoxyphenylacetic acid			
CAS-No. EC-No.	104-01-8 203-166-4 *	Eye Dam. 1; H318	>= 1 - < 3 %
6-Hydroxy-2-oxopyridinium chloride			
CAS-No.	10357-84-3	Skin Irrit. 2; Eye Irrit. 2;	>= 1 - < 10

EC-No.	233-777-1 *	STOT SE 3; H315, H319, H335	%
Barium nitrate			
CAS-No. EC-No. Index-No.	10022-31-8 233-020-5 056-002-00-7 *	Ox. Sol. 2; Acute Tox. 3; Acute Tox. 4; Eye Irrit. 2; H272, H301, H332, H319	>= 1 - < 10 %
4-Amino-N,N-dimethylaniline			
CAS-No. EC-No. Index-No.	99-98-9 202-807-5 612-031-00-2 *	Acute Tox. 2; Acute Tox. 3; Acute Tox. 1; H300, H331, H310	>= 1 - < 10 %
Pyrrole-2-carboxylic acid			
CAS-No. EC-No.	634-97-9 211-221-9 *	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
Quinoline-4-carboxylic acid			
CAS-No. EC-No.	486-74-8 207-640-1 *	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
butanedione			
CAS-No. EC-No.	431-03-8 207-069-8 *	Flam. Liq. 2; Acute Tox. 4; Acute Tox. 3; Skin Irrit. 2; Eye Dam. 1; Skin Sens. 1; STOT RE 2; H225, H302, H331, H315, H318, H317, H373	>= 1 - < 3 %
2-Methylglutaric acid			
CAS-No. EC-No.	18069-17-5 210-521-7 *	Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; H315, H319, H335	>= 1 - < 10 %
Sodium 3-methyl-2-oxovalerate			
CAS-No. EC-No.	3715-31-9 266-503-4 *	Eye Irrit. 2; H319	>= 1 - < 10 %
Manganese(IV) oxide			
CAS-No. EC-No. Index-No.	1313-13-9 215-202-6 025-001-00-3 *	Acute Tox. 4; STOT RE 2; H302, H332, H373	>= 1 - < 10 %
hydroquinone			
CAS-No. EC-No. Index-No.	123-31-9 204-617-8 604-005-00-4	Acute Tox. 4; Eye Dam. 1; Skin Sens. 1B; Muta. 2; Carc. 2; Aquatic Acute 1;	>= 1 - < 2.5 %

Registration number	01-2119524016-51-XXXX	Aquatic Chronic 1; H302, H318, H317, H341, H351, H400, H410 M-Factor - Aquatic Acute: 10	
Benzyl alcohol			
CAS-No. EC-No. Index-No. Registration number	100-51-6 202-859-9 603-057-00-5 01-2119492630-38-XXXX	Acute Tox. 4; Eye Irrit. 2; H302, H332, H319	>= 1 - < 10 %
phenylacetaldehyde			
CAS-No. EC-No.	122-78-1 204-574-5 *	Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1A; Aquatic Chronic 3; H302, H314, H318, H317, H412	>= 1 - < 2.5 %
Pyruvaldehyde			
CAS-No. EC-No.	78-98-8 201-164-8 *	Met. Corr. 1; Acute Tox. 4; Eye Dam. 1; Skin Sens. 1B; Muta. 2; H290, H302, H318, H317, H341	>= 0.1 - < 1 %

*A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, or the annual tonnage does not require a registration.

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Consult a physician. Show this material safety data sheet to the doctor in attendance.First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.After inhalation: fresh air. Call in physician.

In case of skin contact
Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Sulfur oxides
Oxides of phosphorus
Hydrogen chloride gas
Potassium oxides
Sodium oxides
Lithium oxides
Mixture with combustible ingredients.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Use water spray to cool unopened containers.Use water spray to cool unopened containers.Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.Work under hood. Do not inhale substance/mixture.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Keep locked up or in an area accessible only to qualified or authorized persons.
Storage stability Recommended storage temperature
-20 °C
Storage class
Storage class (TRGS 510): 3: Flammable liquids

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

8.2 Exposure controls

Personal protective equipment

Eye/face protection
Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection
The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
protective clothing

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).
required when dusts are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.
Recommended Filter type: Filter type P3

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.
Discharge into the environment must be avoided.
Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Physical state	solid
b)	Color	No data available
c)	Odor	No data available
d)	Melting point/freezing point	No data available
e)	Initial boiling point and boiling range	No data available
f)	Flammability (solid, gas)	No data available
g)	Upper/lower flammability or explosive limits	No data available
h)	Flash point	-4.99 °C
i)	Autoignition temperature	No data available
j)	Decomposition temperature	No data available
k)	pH	No data available
l)	Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m)	Water solubility	No data available
n)	Partition coefficient: n-octanol/water	No data available
o)	Vapor pressure	No data available
p)	Density	No data available
	Relative density	No data available
q)	Relative vapor density	No data available
r)	Particle characteristics	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
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature) .
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Violent reactions possible with:

10.4 Conditions to avoid
Heat, flames and sparks.
Heat, flames and sparks.
no information 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

Mixture

Acute toxicity
Acute toxicity estimate Oral - 1,806 mg/kg
(Calculation method)
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Acute toxicity estimate Inhalation - 4 h - > 5 mg/l - dust/mist(Calculation method)

Symptoms: Possible symptoms:, mucosal irritations
Acute toxicity estimate Dermal - 42 mg/kg
(Calculation method)

Skin corrosion/irritation
Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation
Remarks: Mixture causes serious eye damage.

Respiratory or skin sensitization
Mixture may cause an allergic skin reaction.

Germ cell mutagenicity
Evidence of genetic defects.

Carcinogenicity
Evidence of a carcinogenic effect.

Reproductive toxicity

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

Endocrine disrupting properties

Product:

Assessment	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components

3-Hydroxyphenyl acetate

Acute toxicity
LD50 Oral - 500.1 mg/kg
Inhalation: No data available
Dermal: No data available
LD50 Intraperitoneal - Mouse - 400 mg/kg
Remarks:
Behavioral:Somnolence (general depressed activity).
Behavioral:Tremor.
Behavioral:Ataxia.

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe eye irritation
(Draize Test)

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
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

1-Methyl-6,7-dihydroxy-1,2,3,4-tetrahydroisoquinoline hydrobromide

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

3-Hydroxybenzoic acid

Acute toxicity
LD50 Oral - Mouse - 2,000 mg/kg
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Itaconic acid

Acute toxicity
LD50 Oral - Rat - > 2,000 mg/kg
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Remarks: (External MSDS)
Symptoms: Possible damages:, mucosal irritations
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
Remarks: (IUCLID)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Eye irritation
Remarks: (IUCLID)
Risk of serious damage to eyes.
Eyes - Rabbit
Result: Causes serious eye damage.
(OECD Test Guideline 405)

Respiratory or skin sensitization
Sensitisation test: - Guinea pig
Result: negative
Remarks: (IUCLID)

Germ cell mutagenicity
Test Type: Ames test
Result: negative
Remarks: (IUCLID)

Result: negative
Remarks: (IUCLID)

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Acute oral toxicity - Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Acute inhalation toxicity - Possible damages:, mucosal irritations

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

2-Methylbutyraldehyde

Acute toxicity
LD50 Oral - Rat - male - 6,884 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - 4 h - 50.5 mg/l - vapor
(OECD Test Guideline 403)
LD50 Dermal - Rabbit - male - 5,400 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Eyes - Rabbit
Result: irritating - 8 d
Eyes - Rat
Result: Eye irritation
Remarks: (RTECS)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: positive
(OECD Test Guideline 429)

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

2',4'-Dihydroxyacetophenone

Acute toxicity
LD50 Oral - Rat - 2,830 mg/kg
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Remarks: (RTECS)
Symptoms: Possible damages:, mucosal irritations
Dermal: No data available

Skin corrosion/irritation
Remarks: slight irritation

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe irritations
Remarks: (RTECS)

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Acute oral toxicity - Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Acute inhalation toxicity - Possible damages:, mucosal irritations

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Salicylic acid

Acute toxicity
LD50 Oral - Rat - male - 891 mg/kg
(OECD Test Guideline 401)
Oral: Behavioral:Muscle weakness.
Acute toxicity estimate Oral - 891 mg/kg
(ATE value derived from LD50/LC50 value)
Inhalation: No data available
LD50 Dermal - Rat - male and female - > 2.000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Risk of serious damage to eyes.
(Draize Test)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: Chinese hamster ovary cells
Result: negative
Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Result: negative
Method: OECD Test Guideline 475
Species: Mouse - male - Bone marrow
Result: negative
Method: US-EPA
Species: Mouse - male - Bone marrow
Result: negative

Carcinogenicity
No data available

Reproductive toxicity
Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard
No data available

Salicylamide

Acute toxicity
LD50 Oral - Rat - 980 mg/kg
Remarks: Behavioral:Altered sleep time (including change in righting reflex).
Behavioral:Somnolence (general depressed activity).
Respiratory disorder
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Moderate eye irritation - 48 h

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
Laboratory experiments have shown teratogenic effects.

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

3-hydroxyphenylacetic acid

Acute toxicity
Oral: No data available
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

suberic acid

Acute toxicity
LD50 Oral - Rat - > 2,000 mg/kg
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Moderate eye irritation

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
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

Citraconic acid

Acute toxicity
LD50 Oral - Rat - 1,320 mg/kg
Remarks: Behavioral:Somnolence (general depressed activity).
Behavioral:Tremor.
Gastrointestinal:Ulceration or bleeding from stomach.
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
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

N-Ethyl-2-(isopropyl)-5-methylcyclohexanecarboxamide

Acute toxicity
Oral: No data available
LD50 Oral - 500.1 mg/kg
Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
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

O,O'-Bis(3-aminopropyl)polyethylene glycol

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

2-Oxo-hexanedioic acid

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
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

Indole-3-acetaldehyde sodium bisulfite

Acute toxicity
Oral: No data available
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

(S)-(-)-1-phenylethanol

Acute toxicity
LD50 Oral - Rat - 400 mg/kg
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Remarks: (racemate)
(Lit.)
Inhalation: No data available
LD50 Dermal - Rabbit - 2,500 mg/kg
Remarks: (racemate)
(External MSDS)

Skin corrosion/irritation
Skin - Rabbit
Result: Irritations
(Draize Test)
Remarks: (RTECS)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe irritations
(Draize Test)
Remarks: (RTECS)

Respiratory or skin sensitization
Sensitisation test (Magnusson and Kligman):
Result: negative
Remarks: (racemate)
(External MSDS)

Germ cell mutagenicity
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Remarks: (Lit.)

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Acute oral toxicity - Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

trans-Cinnamaldehyde

Acute toxicity
Oral: No data available
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
Test Type: Hamster
Test system: fibroblast
Remarks: Cytogenetic analysis
Test Type: Hamster
Test system: fibroblast
Remarks: Morphological transformation.
Test Type: Hamster
Test system: ovary
Remarks: Sister chromatid exchange
Species: Mouse
Remarks: Micronucleus test
Species: Rat
Remarks: Micronucleus test

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

pyruvic acid

Acute toxicity
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.
Symptoms: Shortness of breath, Cough, mucosal irritations, Lung edema, Pneumonia, Possible damages:, damage of respiratory tract
Dermal: No data available

Skin corrosion/irritation
Remarks: Causes severe burns.
(ECHA)

Serious eye damage/eye irritation
Remarks: Causes serious eye damage.
(ECHA)

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
Test Type: Ames test
Test system: S. typhimurium
Result: negative
Remarks: (ECHA)

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Acute oral toxicity - If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.
Acute inhalation toxicity - Shortness of breath, Cough, mucosal irritations, Lung edema, Pneumonia, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

adipic acid

Acute toxicity
LD50 Oral - Rat - male and female - 5,560 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - male and female - 4 h - > 7.7 mg/l - dust/mist
(OECD Test Guideline 403)
LD50 Dermal - Rabbit - male and female - > 7,940 mg/kg
Remarks: (40% solution)
(External MSDS)

Skin corrosion/irritation
Skin - Rabbit
Result: slight irritation - 24 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Causes serious eye damage. - 24 h
(OECD Test Guideline 405)

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: negative
Remarks: (ECHA)

Germ cell mutagenicity
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster lung cells
Result: negative
Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: human diploid fibroblasts
Result: negative
Remarks: (ECHA)
Species: Rat - male - Bone marrow
Result: negative
Remarks: (ECHA)

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard
No data available

Azelaic acid

Acute toxicity
LD50 Oral - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 401)
Remarks: (in analogy to similar compounds)
LC50 Inhalation - Rat - male and female - 4 h - > 0.162 mg/l - vapor
Remarks: (in analogy to similar products)
(ECHA)
The value is given in analogy to the following substances: Octanoic acid
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 434)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: stearic acid

Skin corrosion/irritation
Skin - Rabbit
Result: Irritating to skin. - 4 h
(OECD Test Guideline 404)
Remarks: (in analogy to similar products)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Causes serious eye irritation.
Remarks: (in analogy to similar products)
(ECHA)

Respiratory or skin sensitization
Maximization Test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: Ames test
Test system: S. typhimurium
Result: negative

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard
No data available

Vanillin

Acute toxicity
LD50 Oral - Rat - male and female - 3,925 - 3,978 mg/kg
(EC Directive 92/69/EEC B.1 Acute Toxicity (Oral))
Inhalation: No data available
LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation
Skin - Rat
Result: No skin irritation - 24 h
Remarks: (ECHA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Causes serious eye irritation.
(OECD Test Guideline 405)

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Test system: Chinese hamster ovary cells
Result: negative
Method: Mutagenicity (micronucleus test)
Species: Mouse - female - Bone marrow
Result: negative

Carcinogenicity
No data available

Reproductive toxicity
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

methyl acetoacetate

Acute toxicity
LD50 Oral - Rat - male - 2,580 mg/kg
(OECD Test Guideline 401)
Remarks: (ECHA)
Inhalation: No data available
LD50 Dermal - Rat - > 2,000 mg/kg
Remarks: (ECHA)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Eye irritation
(OECD Test Guideline 405)
Remarks: (ECHA)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: Not a skin sensitizer.
(OECD Test Guideline 429)
Remarks: (ECHA)

Germ cell mutagenicity
No data available
Test Type: Ames test
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster fibroblasts
Result: negative

Carcinogenicity
No data available

Reproductive toxicity
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

4-Methoxyphenylacetic acid

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
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

6-Hydroxy-2-oxopyridinium chloride

Acute toxicity
Oral: No data available
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Barium nitrate

Acute toxicity
LD50 Oral - Rat - female - 50 - 300 mg/kg
(OECD Test Guideline 423)
Acute toxicity estimate Inhalation - 1.6 mg/l - dust/mist
(Expert judgment)
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: irritating
(OECD Test Guideline 405)

Respiratory or skin sensitization
Sensitisation test: - Mouse
Result: Does not cause skin sensitization.
(OECD Test Guideline 429)

Germ cell mutagenicity
Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Result: negative

Carcinogenicity
No data available

Reproductive toxicity
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

4-Amino-N,N-dimethylaniline

Acute toxicity
LD50 Oral - Rat - 50 mg/kg
Remarks: Behavioral:Tremor.
Behavioral:Convulsions or effect on seizure threshold.

LC50 Inhalation - 4 h - 0.51 mg/l - dust/mist
LD50 Dermal - Guinea pig - 0.5 mg/kg
LD50 Intraperitoneal - Rabbit - 100 mg/kg
Remarks:
Behavioral:Convulsions or effect on seizure threshold.
Behavioral:Excitement.
LD50 Intraperitoneal - Rat - 21 mg/kg
Remarks:
Behavioral:Convulsions or effect on seizure threshold.
Behavioral:Excitement.
LD50 Intraperitoneal - Mouse - 25 mg/kg
LD50 Intraperitoneal - Guinea pig - 45 mg/kg
Remarks:
Behavioral:Convulsions or effect on seizure threshold.
Behavioral:Excitement.

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

Germ cell mutagenicity
Test Type: Rat
Test system: Liver
Remarks: Unscheduled DNA synthesis
Test Type: Hamster
Test system: Lungs
Remarks: Cytogenetic analysis
Test Type: Ames test
Test system: S. typhimurium

Carcinogenicity
No data available

Reproductive toxicity
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

Pyrrole-2-carboxylic acid

Acute toxicity
Oral: No data available
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Quinoline-4-carboxylic acid

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

butanedione

Acute toxicity
LD50 Oral - Rat - 1,580 mg/kg
Remarks: Behavioral:Somnolence (general depressed activity).
Behavioral:Convulsions or effect on seizure threshold.
(RTECS)
Acute toxicity estimate Oral - 1,580 mg/kg
(Calculation method)
LC50 Inhalation - Rat - 4 h - 2.25 - 5.2 mg/l - vapor
Remarks: (External MSDS)
Symptoms: Possible damages:, Irritation symptoms in the respiratory tract.
Acute toxicity estimate Inhalation - 2.25 mg/l - vapor
(Calculation method)
LD50 Dermal - Rabbit - > 5,000 mg/kg
Remarks: (RTECS)

Skin corrosion/irritation
Skin - Rabbit
Result: Irritations
Remarks: (External MSDS)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe eye irritation
Remarks: (External MSDS)

Respiratory or skin sensitization
May cause allergic skin reaction.

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Acute inhalation toxicity - Possible damages:, Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure
Inhalation - May cause damage to organs through prolonged or repeated exposure.
- Respiratory system

Aspiration hazard
No data available

2-Methylglutaric acid

Acute toxicity
Oral: No data available
Inhalation: Irritating to respiratory system.
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Sodium 3-methyl-2-oxovalerate

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
Remarks: Causes serious eye irritation.
The value is given in analogy to the following substances: 3-methyl-2-oxovaleric acid

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
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

Manganese(IV) oxide

Acute toxicity
Acute toxicity estimate Oral - 500.1 mg/kg
(Expert judgment)
Acute toxicity estimate Inhalation - 1.6 mg/l - dust/mist
(Expert judgment)
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation - 72 h
(OECD Test Guideline 405)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity
No data available

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
Inhalation - May cause damage to organs through prolonged or repeated exposure.
- Brain

Aspiration hazard
No data available

hydroquinone

Acute toxicity
LD50 Oral - Rat - female - 367.3 mg/kg
(OECD Test Guideline 401)
Acute toxicity estimate Oral - 367.3 mg/kg
(ATE value derived from LD50/LC50 value)
Inhalation: No data available
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 24 h
Remarks: (ECHA)

Serious eye damage/eye irritation
Remarks: Causes serious eye damage.
(Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: positive
(OECD Test Guideline 429)

Germ cell mutagenicity
Suspected of causing genetic defects.
Test Type: Ames test
Test system: S. typhimurium
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: Human lymphocytes
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Result: positive
Test Type: Chromosome aberration test in vitro
Test system: Chinese hamster ovary cells
Result: negative
Remarks: (ECHA)
Method: OECD Test Guideline 489
Species: Rat - male and female
Result: negative
Method: OECD Test Guideline 488
Species: Mouse - male
Result: negative
Method: OECD Test Guideline 478
Species: Rat - male
Result: negative
Method: OECD Test Guideline 474
Species: Mouse - male and female - Red blood cells (erythrocytes)
Result: positive
Species: Mouse - male - Red blood cells (erythrocytes)
Result: positive
Remarks: (ECHA)

Carcinogenicity
Suspected of causing cancer.

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard
No data available

Benzyl alcohol

Acute toxicity
LD50 Oral - Rat - male - 1,620 mg/kg
Remarks: (ECHA)
LC50 Inhalation - 4 h - 11 mg/l - dust/mist
LC50 Inhalation - Rat - male and female - 4 h - > 4.178 mg/l - aerosol
(OECD Test Guideline 403)
Remarks: (Regulation (EC) No 1272/2008, Annex VI)
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: irritating
(OECD Test Guideline 405)

Respiratory or skin sensitization
Maximization Test
Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Method: OECD Test Guideline 474
Species: Mouse - male - Red blood cells (erythrocytes)
Result: negative

Carcinogenicity
No data available

Reproductive toxicity
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

phenylacetaldehyde

Acute toxicity
LD50 Oral - Rat - 1,550 mg/kg
(OECD Test Guideline 401)
Inhalation: No data available
LD50 Dermal - Rabbit - > 5,000 mg/kg
Remarks: (RTECS)

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
Test Type: reverse mutation assay
Test system: TA1535
Result: negative
Test Type: reverse mutation assay
Test system: E. coli
Result: negative

Carcinogenicity
No data available

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard
No data available

Pyruvaldehyde

Acute toxicity
LD50 Oral - Rat - male and female - 1,380 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - male and female - 4 h - > 13.6 mg/l - Aerosol
(OECD Test Guideline 403)
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin-irritant effect in animal experiments. - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Irreversible effects on the eye
(OECD Test Guideline 405)

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: positive
(OECD Test Guideline 406)
Remarks: The value is given in analogy to the following substances: Glyoxazal

Germ cell mutagenicity
Suspected of causing genetic defects.

Carcinogenicity
No data available

Reproductive toxicity
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

SECTION 12: Ecological information

12.1 Toxicity

Mixture
No data available

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.
This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties
Product:

Assessment	:	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects
Very toxic to aquatic life with long lasting effects.

Components

3-Hydroxyphenyl acetate

No data available

1-Methyl-6,7-dihydroxy-1,2,3,4-tetrahydroisoquinoline hydrobromide
No data available

3-Hydroxybenzoic acid

Toxicity to algae	Growth inhibition EC50 - Scenedesmus quadricauda (Green algae) - > 10 mg/l - 13 d

Itaconic acid

Toxicity to fish	LC50 - Oncorhynchus mykiss (rainbow trout) - 190 mg/l - 24 h Remarks: (IUCLID)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 240 mg/l - 24 h Remarks: (IUCLID)
Toxicity to algae	IC50 - Desmodesmus subspicatus (green algae) - 47 mg/l - 72 h Remarks: (IUCLID)

2-Methylbutyraldehyde

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 9.9 mg/l - 96 h Remarks: (ECOTOX Database)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 7.2 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 123 mg/l - 72 h (OECD Test Guideline 201)

2',4'-Dihydroxyacetophenone

No data available

Salicylic acid

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,370 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: Sodium salicylate
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 870 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	Growth inhibition ErC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - Pseudomonas putida - 380 mg/l - 16 h Remarks: (ECHA) The value is given in analogy to the following substances: methyl salicylate
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	NOEC - Daphnia magna (Water flea) - 10 mg/l - 21 d (OECD Test Guideline 202)

Salicylamide

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 101 mg/l - 96 h

3-hydroxyphenylacetic acid
No data available

suberic acid
No data available

Citraconic acid
No data available

N-Ethyl-2-(isopropyl)-5-methylcyclohexanecarboxamide
No data available

O,O'-Bis(3-aminopropyl)polyethylene glycol
No data available

2-Oxo-hexanedioic acid

No data available

Indole-3-acetaldehyde sodium bisulfite
No data available

(S)-(-)-1-phenylethanol

Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 102 mg/l - 48 h Remarks: (racemate) (External MSDS)

trans-Cinnamaldehyde
No data available

pyruvic acid

No data available

adipic acid

Toxicity to daphnia and other aquatic invertebrates	static test LC50 - Daphnia magna (Water flea) - 46 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 64.5 mg/l - 72 h (OECD Test Guideline 201)
	static test NOEC - Pseudokirchneriella subcapitata (green algae) - 40.6 mg/l - 72 h

	(OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - > 100 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	flow-through test NOEC - Daphnia magna (Water flea) - 6.3 mg/l - 21 d (OECD Test Guideline 211)

Azelaic acid

Toxicity to fish	semi-static test LC50 - Oryzias latipes - > 16 mg/l - 96 h (OECD Test Guideline 203) Remarks: (in analogy to similar products) The value is given in analogy to the following substances: Decanoic acid
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - > 20 mg/l - 48 h (OECD Test Guideline 202) Remarks: (in analogy to similar products) The value is given in analogy to the following substances: Decanoic acid
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - > 67 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC10 - Pseudomonas putida - 912 mg/l - 18 h (ISO 10712)
Toxicity to fish(Chronic toxicity)	flow-through test LC50 - Danio rerio (zebra fish) - 9.8 mg/l - 28 d Remarks: (ECHA) (in analogy to similar products) The value is given in analogy to the following substances: lauric acid
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 0.2 mg/l - 21 d (OECD Test Guideline 211) Remarks: (in analogy to similar products) The value is given in analogy to the following substances: Decanoic acid
	semi-static test EC50 - Daphnia magna (Water flea) - 0.51 mg/l - 21 d (OECD Test Guideline 211) Remarks: (in analogy to similar products) The value is given in analogy to the following substances: Decanoic acid

Vanillin

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 57 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 36.6 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 120 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	IC50 - microorganisms - 163 mg/l - 40 h Remarks: (External MSDS)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 5.9 mg/l - 21 d (OECD Test Guideline 202)
	semi-static test EC50 - Daphnia magna (Water flea) - 16 mg/l - 21 d (OECD Test Guideline 202)

methyl acetoacetate

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - > 111.4 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)

4-Methoxyphenylacetic acid
No data available

6-Hydroxy-2-oxopyridinium chloride
No data available

Barium nitrate
No data available

4-Amino-N,N-dimethylaniline
No data available

Pyrrole-2-carboxylic acid
No data available

Quinoline-4-carboxylic acid

No data available

butanedione

Toxicity to fish	LC50 - Leuciscus idus (Golden orfe) - 46 - 100 mg/l - 96 h Remarks: (External MSDS)
Toxicity to bacteria	Remarks: (Hommel)

2-Methylglutaric acid

No data available

Sodium 3-methyl-2-oxovalerate

No data available

Manganese(IV) oxide

No data available

hydroquinone

Toxicity to fish	flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - 0.638 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 0.134 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 0.33 mg/l - 72 h (OECD Test Guideline 201)
	static test NOEC - Pseudokirchneriella subcapitata - 0.019 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Pimephales promelas (fathead minnow) - >= 0.1 mg/l - 32 d (OECD Test Guideline 210)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test LC50 - Daphnia magna (Water flea) - 0.061 mg/l - 21 d (OECD Test Guideline 211)

Benzyl alcohol

Toxicity to fish	static test LC50 - Pimephales promelas (fathead minnow) - 460 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - 230 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 700 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 51 mg/l - 21 d (OECD Test Guideline 211)

phenylacetaldehyde

Toxicity to fish	LC50 - Danio rerio (zebra fish) - > 6.2 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 20 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 1.6 mg/l - 72 h (OECD Test Guideline 201)

Pyruvaldehyde

Toxicity to fish	static test LC50 - Leuciscus idus (Golden orfe) - ca. 1,000 mg/l - 96 h (DIN 38412)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 404 mg/l - 48 h (Regulation (EC) No. 440/2008, Annex, C.2)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 731.5 mg/l - 72 h (DIN 38412)
Toxicity to bacteria	static test EC50 - Pseudomonas putida - 11 mg/l - 17 h (DIN 38421 TEIL 8)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 3316 IMDG: 3316 IATA: 3316

14.2 UN proper shipping name

ADR/RID: CHEMICAL KIT (butanedione)
IMDG: CHEMICAL KIT (butanedione)
IATA: Chemical kit (butanedione)

14.3 Transport hazard class(es)

ADR/RID: 9 IMDG: 9 IATA: 9

14.4 Packaging group

ADR/RID: II IMDG: II IATA: II

14.5 Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

14.6 Special precautions for user

Further information : No data available

SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Authorisations and/or restrictions on use

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.	H1	ACUTE TOXIC
	E2	ENVIRONMENTAL HAZARDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

H225	Highly flammable liquid and vapor.
H272	May intensify fire; oxidizer.
H290	May be corrosive to metals.
H300	Fatal if swallowed.
H301	Toxic if swallowed.
H302	Harmful if swallowed.

H310	Fatal in contact with skin.
H314	Causes severe skin burns and eye damage.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H341	Suspected of causing genetic defects.
H351	Suspected of causing cancer.
H361d	Suspected of damaging the unborn child.
H373	May cause damage to organs through prolonged or repeated exposure if inhaled.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
H411	Toxic to aquatic life with long lasting effects.
H412	Harmful to aquatic life with long lasting effects.

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

Classification of the mixture		Classification procedure:
Acute Tox.4	H302	Calculation method
Acute Tox.1	H310	Calculation method
Skin Irrit.2	H315	Calculation method
Eye Dam.1	H318	Calculation method
Skin Sens.1	H317	Calculation method
Muta.2	H341	Calculation method
Carc.2	H351	Calculation method
Aquatic Chronic2	H411	Calculation method

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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.