

Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)
Classifications according to Regulation (EC) No 1272/2008.
Printdate 16 Aug 2022

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product name:

3-(4-tert-Butylphenyl)isobutyraldehyde

1.1. Catalog No.:

677066

1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical
uses: R&D

1.3. Uses advised against:

HPC Standards GmbH
Am Wieseneck 7

04451 Cunnersdorf
Deutschland

Tel. +49 34291 3372-36
Fax. +49 34291 3372-39
contact@hpc-standards.com

1.4. Emergency telephone number

HPC Standards Tel. +49 34291 3372-36
This number is only available during office hours.

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008
Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Skin sensitisation (Category 1), H317
Reproductive toxicity (Category 2), H361
Chronic aquatic toxicity (Category 2), H411 Classification according to EU Directives 67/548/EEC or 1999/45/EC
Xn, N Harmful, Dangerous for the environment
R22, R38, R43, R51/53, R62

2.2. Label elements

2.2.1. Pictogram



2.2.2.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram Signal word Warning

Hazard statement(s)

H302 Harmful if swallowed.

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H361 Suspected of damaging fertility or the unborn child.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201 Obtain special instructions before use.

P273 Avoid release to the environment.

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.

P391 Collect spillage.

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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula : C₁₄H₂₀O

Molecular weight : 204,3 g/mol

CAS-No. : 80-54-6

EC-No. : 201-289-8

Hazardous ingredients according to Regulation (EC) No 1272/2008

Component Classification Concentration

2-(4-tert-Butylbenzyl)propionaldehyde

CAS-No.

EC-No.

80-54-6

201-289-8

Acute Tox. 4; Skin Irrit. 2; Skin

Sens. 1; Repr. 2; Aquatic

Chronic 2; H302, H315, H317,

H361, H411

<= 100 %

Hazardous ingredients according to Directive 1999/45/EC

Component Classification Concentration

2-(4-tert-Butylbenzyl)propionaldehyde

CAS-No.

EC-No.

80-54-6

201-289-8

Xn, N, R22 - R38 - R43 -

R51/53 - R62

<= 100 %

3.1.1. Formula

C₁₄H₂₀O

3.1.2. Molecular Weight (g/mol)

204.31

3.1.3. CAS-No.

80-54-6

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.

Evacuate personnel to safe areas.

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.

6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

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.

Recommended storage temperature 2 - 8 °C

Air sensitive. Store under inert gas.

Storage class (TRGS 510): Combustible liquids

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

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, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

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).

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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance Form: clear, viscous liquid

Colour: colourless

b) Odour No data available

c) Odour Threshold No data available

d) pH No data available

e) Melting point/freezing point

Melting point/freezing point: < -19,99 °C at 1.013,250 hPa - OECD Test

Guideline 102

f) Initial boiling point and

boiling range

279,4 - 285,5 °C at 1.013,250 hPa - OECD Test Guideline 103

g) Flash point 113,75 - 114,25 °C - closed 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) Vapour pressure No data available

l) Vapour density No data available

m) Relative density ca.0,946 g/cm³ at 20 °C

n) Water solubility ca.0,045 g/l at 20 °C - OECD Test Guideline 105 - slightly soluble

o) Partition coefficient: noctanol/

water

log Pow: 4,73 at 25 °C

p) Auto-ignition

temperature

242 °C at 1.010 hPa

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

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

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

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 1.390 mg/kg

(OECD Test Guideline 401)
LD50 Dermal - Rat - male and female - > 2.000 mg/kg
(OECD Test Guideline 402)
Skin corrosion/irritation
Skin - Rabbit
Result: Skin irritation - 4 h
(OECD Test Guideline 404)
Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
Respiratory or skin sensitisation
Maximisation Test (GPMT) - Guinea pig Result: May cause sensitisation by skin contact.
(OECD Test Guideline 406)
Germ cell mutagenicity
Ames test
Salmonella typhimurium
Result: negative
OECD Test Guideline 474
Mouse - male and female
Result: negative
Carcinogenicity
IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
Reproductive toxicity
Reproductive toxicity - Rat - Oral
Paternal Effects: Testes, epididymis, sperm duct.
Suspected human reproductive toxicant
Developmental Toxicity - Rabbit - Oral
Specific Developmental Abnormalities: Musculoskeletal system.
Specific target organ toxicity - single exposure
No data available
Specific target organ toxicity - repeated exposure
No data available
Aspiration hazard
No data available
Additional Information
Repeated dose toxicity - Rat - male and female - Oral - No observed adverse effect level - 25 mg/kg
RTECS: MW4895000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity
Toxicity to fish flow-through test LC50 - Danio rerio (zebra fish) - 2,04 mg/l - 96 h
(OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates
Immobilization EC50 - Daphnia magna (Water flea) - 9,84 mg/l - 48 h
(OECD Test Guideline 202)
Toxicity to algae Growth inhibition EC50 - Desmodesmus subspicatus (green algae) - ca. 32,5 mg/l - 72 h
(OECD Test Guideline 201)
12.2 Persistence and degradability
Biodegradability aerobic - Exposure time 28 d
Result: 80,7 % - Readily biodegradable
(OECD Test Guideline 301B)
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.
12.6 Other adverse effects
Toxic to aquatic life with long lasting effects

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product

14. TRANSPORT INFORMATION

14.1 UN number

ADR/RID: 3082 IMDG: 3082 IATA: 3082

14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (2-(4-tert-Butylbenzyl)propionaldehyde)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (2-(4-tert-Butylbenzyl)propionaldehyde)

IATA: Environmentally hazardous substance, liquid, n.o.s. (2-(4-tert-Butylbenzyl)propionaldehyde)

14.3 Transport hazard class(es)

ADR/RID: 9 IMDG: 9 IATA: 9

14.4 Packaging group

ADR/RID: III IMDG: III IATA: III

14.5 Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: yes

14.6 Special precautions for user

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids

15. REGULATORY INFORMATION

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

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

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

16. OTHER INFORMATION

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. For lab use only!