

tert-Butyl bromoacetate

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

1.1. Product identifier

Trade name

tert-Butyl bromoacetate

CAS number

5292-43-3

EC number

226-133-6

Synonyms

Bromoacetic acid tert-butyl ester, t-Butyl bromoacetate, tert-Butyl 2-bromoacetate

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

Relevant identified uses

Research and development.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Address

Molekula Ltd, Lingfield Way, Darlington, DL1 4XX Darlington United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

<u>Email</u>

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)



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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Flammable liquids, hazard category 3

Acute toxicity, oral, hazard category 4

Skin corrosion, hazard category 1B

Specific Target Organ Toxicity — Single exposure, hazard category 3 - respiratory tract irritation

Hazard statements

H226, H302, H314, H335

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms







Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H335 May cause respiratory irritation.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

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

P302 + P352 IF ON SKIN: Wash with plenty of water/.

P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.

P304+P341 IF INHALED: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3. Other hazards

No data available

According to Regulation (EC) No 2020/878



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SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrase M factor acute M factor chronic	Note
tert-butyl bromoacetate	5292-43-3 226-133-6 -	100%	Flam. Liq. 3, Acute Tox. 4 - oral, Skin Corr. 1B, STOT SE 3 - resp. tract irrit.	H226, H302, H314, H335 -	-

Molecular weight

195.05

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary.

Skin contact

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor.

Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

Ingestion

IF SWALLOWED: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only if the persons are fully conscious and awake).

Information for doctors

No data available.



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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. Causes burns by all exposure routes.

See section 11 for more detailed information on health effects and symptoms.

Inhalation

Single exposure may cause the following adverse effects: Causes severe burns. Difficulty in breathing. Unconsciousness, possibly death.

Skin contact

Single exposure may cause the following adverse effects: Causes severe burns. Blistering may occur. May be absorbed in the body and cause dizziness, nausea and vomiting. Unconsciousness, death.

Eye contact

Single exposure may cause the following adverse effects: Causes serious eye damage. Unconsciousness, possibly death.

Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury. Unconsciousness, possibly death.

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

Treat symptomatically. Immediately call a POISON CENTER/doctor.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

Unsuitable extinguishing media

No specific fire fighting procedure given.

5.2. Special hazards arising from the substance or mixture

Specific hazards: Highly flammable Corrosive.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO2). Hydrogen bromide (HBr).

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Prevent skin contact by maintaining a safe distance and by wearing suitable protective equipment/ clothing. Cool containers exposed to heat with water spray and remove container, if no risk is involved.



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SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Do not breathe vapour/spray. Avoid contact with skin and eyes. For personal protection, see section 8.

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground. Risk of explosion.

6.3. Methods and material for containment and cleaning up

Collect with absorbent, non-combustible material into suitable containers.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2. Work under hood Take action to prevent static discharges. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use.

7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container.

Store at ambient temperature.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No data available

8.2. Exposure controls

Personal Protective Equipment Symbols









Eye / face protection

Wear eye protection.



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Hand protection

Wear protective gloves. Recommended gloves: Butyl rubber.

Glove Thickness: 0.7mm Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

Environmental exposure controls

Avoid discharge into drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Liquid

Colour

Clear, yellowish liquid.

Odour

No data available

Melting point / freezing point

No data available

Boiling point or initial boiling point and boiling range

No data available

Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

~ 49 °C

Method

CC (Closed cup).

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Auto-ignition temperature

No data available

Decomposition temperature

No data available

pН

No data available

Kinematic viscosity

No data available

Solubility

Soluble in water.

Partition coefficient n-octanol/water

No data available

Vapour pressure

No data available

Density and/or relative density

1.321 g/cm³

Method

(25°C)

Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2. Chemical stability

Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidising agents. Bases.

10.4. Conditions to avoid

Heating.

According to Regulation (EC) No 2020/878



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10.5. Incompatible materials

Strong oxidising agents.

10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008 Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Test animals
tert-butyl bromoacetate 5292-43-3 / 226-133-6	Acute Toxicity (Oral LD50):	400mg/kg	Rat
tert-butyl bromoacetate 5292-43-3 / 226-133-6	Acute Toxicity (Dermal LD50):	> 2,000mg/kg	Rat

Skin corrosion/irritation

Product / Substance name CAS / EC no.	Result	Duration of exposure	Species
tert-butyl bromoacetate 5292-43-3 / 226-133-6	Causes skin burns.	4 hours	Rabbit

Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result
tert-butyl bromoacetate 5292-43-3 / 226-133-6	Causes serious eye damage.

Respiratory or skin sensitisation

Product / Substance name CAS / EC no.	Result	Species
tert-butyl bromoacetate 5292-43-3 / 226-133-6	Negative.	Guinea Pig

Germ cell mutagenicity



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Product / Substance name CAS / EC no.	Result	Method / Guideline
tert-butyl bromoacetate 5292-43-3 / 226-133-6	Negative.	(OECD Test Guideline 471)

Aspiration hazard

Based on available data, the classification criteria are not met.

11.2. Information on other hazards

No data available

SECTION 12: Ecological information

12.1. Toxicity

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

No data available

12.6. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

SECTION 14: Transport information

14.1. UN number

2920



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14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

CORROSIVE LIQUID, FLAMMABLE, N.O.S. (tert-Butyl bromoacetate)

IMDG proper shipping name

CORROSIVE LIQUID, FLAMMABLE, N.O.S. (tert-Butyl bromoacetate)

IATA proper shipping name

Corrosive liquid, flammable, n.o.s. (tert-Butyl bromoacetate)

14.3. Transport hazard class(es)

Label

ADR/RID/ADN



IMDG



IATA



ADR / RID Class

R

ADR / RID Classification code

CF1

ADR / RID hazard identification number

83

IMDG Class

8 (3)

IATA Class

8 (3)



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ADN Class

8

ADN Class Code

CF1

14.4. Packing group

ADR / RID / ADN: II IMDG: II

IATA: II

14.5. Environmental hazards

IMDG EmS

F-E, S-C

14.6. Special precautions for user

Tunnel restriction code: D/E Transport category: 2

14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC02

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture <u>EU regulations</u>

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

This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

National regulations

No data available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Phrase meaning

Flam. Liq. 3 - Flammable liquids, hazard category 3

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

Skin Corr. 1B - Skin corrosion, hazard category 1B

STOT SE 3 - resp. tract irrit. - Specific Target Organ Toxicity — Single exposure, hazard category

3 - respiratory tract irritation

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H335 May cause respiratory irritation.