according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



(R)-1-[3,5-Bis(trifluoromethyl)phenyl]ethanol ≥99 %

article number: 7481 date of compilation: 2020-12-22 Version: **3.0 en** Revision: 2024-03-03

Replaces version of: 2021-12-20

Version: (2)

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

Product identifier 1.1

Identification of the substance (R)-1-[3,5-Bis(trifluoromethyl)phenyl]ethanol

≥99 %

Article number 7481

It is not required to list the identified uses be-Registration number (REACH)

cause the substance is not subject to registration

according to REACH (< 1 t/a).

CAS number 127852-28-2

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

Relevant identified uses: Laboratory chemical

Laboratory and analytical use

Uses advised against: Do not use for private purposes (household).

Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG Schoemperlenstr. 3-5 D-76185 Karlsruhe Germany

Telephone:+49 (0) 721 - 56 06 0 **Telefax:** +49 (0) 721 - 56 06 149 e-mail: sicherheit@carlroth.de Website: www.carlroth.de

Competent person responsible for the safety data Department Health, Safety and Environment

sheet:

e-mail (competent person): sicherheit@carlroth.de

1.4 **Emergency telephone number**

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Centre Beaumont Hospital	Beaumont Road	Dublin 9	+353 1 809 2166	https:// www.poisons.ie/

SECTION 2: Hazards identification

Classification of the substance or mixture 2.1

Classification according to Regulation (EC) No 1272/2008 (CLP)

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
3.10	Acute toxicity (oral)	4	Acute Tox. 4	H302

For full text of abbreviations: see SECTION 16

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2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word Warning

Pictograms

GHS07



Hazard statements

H302 Harmful if swallowed

Precautionary statements

Precautionary statements - response

P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell

Labelling of packages where the contents do not exceed 125 ml

Signal word: Warning

Symbol(s)



2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \geq 0,1%.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance (R)-1-[3,5-Bis(trifluoromethyl)phenyl]ethanol

Molecular formula $C_{10}H_8F_6O$ Molar mass $258,2\,^9I_{mol}$ CAS No 127852-28-2

Substance, Specific Conc. Limits, M-factors, ATE

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	>300 ^{mg} / _{kg}	oral

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SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

Rinse mouth with water (only if the person is conscious). Call a doctor.

4.2 Most important symptoms and effects, both acute and delayed

Vomiting

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

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

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

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SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid contact with skin, eyes and clothes. Do not breathe dust.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid dust formation.

Measures to prevent fire as well as aerosol and dust generation

Removal of dust deposits.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

7.3 Specific end use(s)

No information available.

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SECTION 8: Exposure controls/personal protection

8.1 **Control parameters**

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Coun	Name of agent	CAS No	Identifi- er	TWA [mg/ m³]	STEL [mg/ m³]	Ceil- ing-C [mg/ m³]	Nota- tion	Source
IE	dusts, non-specific		OELV	10			i	S.I. No. 619 of 2001
IE	dusts, non-specific		OELV	4			r	S.I. No. 619 of 2001

Notation

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

Inhalable fraction

Respirable fraction

STEL

Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)
Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified) TWA

8.2 **Exposure controls**

Individual protection measures (personal protective equipment)

Eye/face protection





Use safety goggle with side protection.

Skin protection





hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

type of material

NBR (Nitrile rubber)

material thickness

>0,11 mm

breakthrough times of the glove material

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>480 minutes (permeation: level 6)

other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection





Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P2 (filters at least 94 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state solid

Form powder, crystalline

Colour whitish - cream
Odour characteristic

Melting point/freezing point 53 – 58 °C

Boiling point or initial boiling point and boiling

range

not determined

Flammability this material is combustible, but will not ignite

readily

Lower and upper explosion limit not determined
Flash point not applicable
Auto-ignition temperature not determined
Decomposition temperature not relevant
pH (value) not applicable
Kinematic viscosity not relevant

Solubility(ies)

Water solubility not determined

Partition coefficient

Partition coefficient n-octanol/water (log value): 3,514

Vapour pressure not determined

Density and/or relative density

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Density not determined

Relative vapour density Information on this property is not available.

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard

classes:

hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics: There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

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

Classification according to GHS (1272/2008/EC, CLP)

Acute toxicity

Harmful if swallowed.

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

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Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

If swallowed

vomiting, abdominal pain, nausea

• If in eyes

Data are not available.

If inhaled

Data are not available.

• If on skin

Data are not available.

Other information

none

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0.1\%$.

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

12.2 Persistence and degradability

Theoretical Oxygen Demand: $1,425 \frac{mg}{mg}$ /_{mg} Theoretical Carbon Dioxide: $1,705 \frac{mg}{mg}$ /_{mg}

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3,514

12.4 Mobility in soil

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Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0.1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

Properties of waste which render it hazardous

HP 6 acute toxicity

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

14.1	UN number or ID number	not subject to transport regulations
		, i 3

14.2 UN proper shipping name not assigned

14.3 Transport hazard class(es) none

14.4 Packing group not assigned

14.5 Environmental hazards non-environmentally hazardous acc. to the dan-

gerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

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14.8 Information for each of the UN Model Regulations

International Maritime Dangerous Goods Code (IMDG) - Additional information

Not subject to IMDG.

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

Not subject to ICAO-IATA.

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list Not listed.

Seveso Directive

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

Deco-Paint Directive

VOC content	0 %
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Industrial Emissions Directive (IED)

VOC content	0 %

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

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

not listed

Water Framework Directive (WFD)

List of pollutants (WFD)					
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks	
(R)-1-[3,5- Bis(trifluoromethyl)phenyl]ethan- ol	Organohalogen compounds and substances which may form such compounds in the aquatic envir- onment		a)		

Legend

a) Indicative list of the main pollutants

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Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

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

not listed

Regulation on persistent organic pollutants (POP)

not listed

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
VN	NCI	substance is listed

Legend

NCI National Chemical Inventory

15.2 Chemical safety assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes
15.1		National inventories	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

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Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
ED	Endocrine disruptor
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regula- tions concerning the International carriage of Dangerous goods by Rail)
S.I. No. 619 of 2001	Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001
STEL	Short-term exposure limit
SVHC	Substance of Very High Concern
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

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

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H302	Harmful if swallowed.

Disclaimer

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

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