acc. to Regulation (EC) No. 1907/2006 (REACH)



4-(2-Aminoethyl)benzenesulfonyl fluoride hydrochloride, Pefabloc® SC-Protease Inhibitor ≥95 %, for biochemistry

date of compilation: 2015-09-22 Revision: 2024-03-02 article number: A154 Version: 4.0 en

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Version: (3)

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

1.1 **Product identifier**

Identification of the substance 4-(2-Aminoethyl)benzenesulfonyl fluoride hy-

drochloride, Pefabloc® SC-Protease Inhibitor

≥95 %, for biochemistry

Article number A154

EC number 608-547-2 CAS number 30827-99-7

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

Relevant identified uses: Laboratory chemical

Laboratory and analytical use

Uses advised against: Do not use for products which come into direct

contact with the skin. Do not use for private purposes (household). Food, drink and animal feed-

ingstuffs.

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 Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	ction Hazard class		Hazard class and category	Hazard statement
3.2	2 Skin corrosion/irritation		Skin Corr. 1C	H314
3.3	Serious eye damage/eye irritation	1	Eye Dam. 1	H318

For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

Skin corrosion produces an irreversible damage to the skin; namely, visible necrosis through the epidermis and into the dermis.

2.2 Label elements

Labelling

Signal word Danger

Pictograms

GHS05



Hazard statements

H314 Causes severe skin burns and eye damage

Precautionary statements

Precautionary statements - prevention

P280 Wear protective gloves/eye protection

Precautionary statements - response

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

with water

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact

lenses, if present and easy to do. Continue rinsing

P310 Immediately call a POISON CENTER/doctor

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%.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance 4-(2-Aminoethyl)benzenesulfonyl fluoride hydro-

chloride

Molecular formula $C_8H_{10}FNO_2S \cdot HCI$

 Molar mass
 239,7 9/mol

 CAS No
 30827-99-7

 EC No
 608-547-2

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off immediately all contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

After contact with skin, wash immediately with plenty of water. Immediate medical treatment required because corrosive injuries that are not treated are hard to cure.

Following eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist. Protect uninjured eye.

Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately. If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects).

4.2 Most important symptoms and effects, both acute and delayed

Corrosion, Risk of blindness, Gastric perforation, Risk of serious damage to eyes

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media



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Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings! water, foam, alcohol resistant 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: Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulphur oxides (SOx)

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. Wear full chemical protective clothing.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Use personal protective equipment as required. 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.

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.

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SECTION 7: Handling and storage

Precautions for safe handling 7.1

Handle and open container with care. Avoid dust formation. Clear contaminated areas thoroughly.

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.

Conditions for safe storage, including any incompatibilities 7.2

Store in a dry place. Keep in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Protect against external exposure, such as

high temperatures

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 4 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 **Control parameters**

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Coun try	Name of agent	CAS No	Identifi- er	TWA [mg/ m³]	STEL [mg/ m³]	Ceil- ing-C [mg/ m³]	Nota- tion	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

Notation

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

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

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8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection





Use safety goggle with side protection. Wear face protection.

Skin protection





hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. 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 quide.

type of material

NBR (Nitrile rubber)

material thickness

>0,11 mm

breakthrough times of the glove material

>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). P1 (filters at least 80 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

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range

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state solid

Form powder, crystalline
Colour white - light beige

Odour odourless

Melting point/freezing point 174 – 178 °C

Boiling point or initial boiling point and boiling 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 $\sim 10^{9}/_{l}$ at 20 °C

Partition coefficient

Partition coefficient n-octanol/water (log value): this information is not available

Vapour pressure not determined

Density and/or relative density

Density not determined

Relative vapour density Information on this property is not available.

Bulk density ~200 kg/_{m³}

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

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

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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, Strong alkali

10.4 Conditions to avoid

Keep away from heat.

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 toxicological effects

Classification acc. to GHS

Acute toxicity

Shall not be classified as acutely toxic.

Skin corrosion/irritation

Causes severe skin burns and eye damage.

Serious eye damage/eye irritation

Causes serious eye damage.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

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).

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Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

If swallowed

If swallowed danger of perforation of the esophagus and the stomach (strong corrosive effects)

• If in eyes

causes burns, Causes serious eye damage, risk of blindness

If inhaled

Inhalation of dust may cause irritation of the respiratory system

• If on skin

causes severe burns, causes poorly healing wounds

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 (without nitrification): 1,368 $^{\rm mg}/_{\rm mg}$ Theoretical Oxygen Demand (with nitrification): 1,635 $^{\rm mg}/_{\rm mg}$ Theoretical Carbon Dioxide: 1,469 $^{\rm mg}/_{\rm mg}$

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

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.

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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

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. 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 4 irritant - skin irritation and eye damage

HP8 corrosive

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

ADRRID UN 3261
IMDG-Code UN 3261
ICAO-TI UN 3261

14.2 UN proper shipping name

ADRRID CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. IMDG-Code CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.

ICAO-TI Corrosive solid, acidic, organic, n.o.s.

Technical name 4-(2-Aminoethyl)benzenesulfonyl fluoride hydro-

chloride

14.3 Transport hazard class(es)

ADRRID 8
IMDG-Code 8
ICAO-TI 8

14.4 Packing group

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14.5	Environmental hazards	non-environmentally hazardous acc. to the dangerous goods regulations
	ICAO-TI	III
	IMDG-Code	III
	ADRRID	III

14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR)Additional information

IIIIOIIIIacioii	
Proper shipping name	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.
Particulars in the transport document	UN3261, CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S., (4-(2-Aminoethyl)benzenesulfonyl fluoride hydrochloride), 8, III, (E)
Classification code	C4
Danger label(s)	8
Special provisions (SP)	274
F () (FO)	E4

Emergency Action Code	2X
Hazard identification No	80
Tunnel restriction code (TRC)	E
Transport category (TC)	3
Limited quantities (LQ)	5 kg
Excepted quantities (EQ)	E1
Special provisions (SP)	2/4

Regulations concerning the International Carriage of Dangerous Goods by Rail (RID)Additional information

Classification code	C4
Danger label(s)	8



Special provisions (SP)	274
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
Transport category (TC)	3
Hazard identification No	80

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International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.

Particulars in the shipper's declaration UN3261, CORROSIVE SOLID, ACIDIC, ORGANIC,

N.O.S., (4-(2-Aminoethyl)benzenesulfonyl fluoride

hydrochloride), 8, III

Marine pollutant

Danger label(s) 8



Special provisions (SP) 223, 274

Excepted quantities (EQ) E1
Limited quantities (LQ) 5 kg
EmS F-A, S-B

Stowage category A

Segregation group 1 - Acids

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

Proper shipping name Corrosive solid, acidic, organic, n.o.s.

Particulars in the shipper's declaration UN3261, Corrosive solid, acidic, organic, n.o.s., (4-

(2-Aminoethyl)benzenesulfonyl fluoride hydro-

chloride), 8, III

Danger label(s) 8



Special provisions (SP)

Excepted quantities (EQ)

Limited quantities (LQ)

5 kg

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)

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

Name of substance	Name acc. to inventory	CAS NO	Listea in	Remarks
4-(2-Aminoethyl)benzenesulfonyl fluoride hydrochloride	Organohalogen compounds and substances which may form such compounds in the aquatic envir- onment		a)	

Legend

a) Indicative list of the main pollutants

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

National regulations(GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

Restrictions according to GB REACH, Annex 17

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.

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National inventories

Country	Inventory	Status
CN	IECSC	substance is listed
NZ	NZIoC	substance is listed
TW	TCSI	substance is listed
VN	NCI	substance is listed

Legend

Inventory of Existing Chemical Substances Produced or Imported in China National Chemical Inventory
New Zealand Inventory of Chemicals IECSC

NZIoC TCSI Taiwan Chemical Substance 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
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

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)	
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)	
Ceiling-C	Ceiling value	
DGR	Dangerous Goods Regulations (see IATA/DGR)	
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an ident fier of substances commercially available within the EU (European Union)	
ED	Endocrine disruptor	
EH40/2005	EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-licence/)	
EINECS	European Inventory of Existing Commercial Chemical Substances	
ELINCS	European List of Notified Chemical Substances	
EmS	Emergency Schedule	
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)	
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations	

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Abbr.	Descriptions of used abbreviations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
STEL	Short-term exposure limit
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

Key literature references and sources for data

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
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.

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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