

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

Calconcarboxylic acid, Practical grade

Version number: GHS 1.0 Date of compilation: 2023-12-30

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

1.1 **Product identifier**

Identification of the substance Calconcarboxylic acid, Practical grade

CAS number 3737-95-9

Alternative name(s) Patton and Reeder's reagent, Practical grade

Alternative number(s) **GRM921**

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

Relevant identified uses Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

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ing office hours: Mon-Fri 09:00 AM - 05:00 PM

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Category	Hazard class and cat- egory	Hazard state- ment
3.2	skin corrosion/irritation	2	Skin Irrit. 2	H315
3.3	serious eye damage/eye irritation	2	Eye Irrit. 2	H319
3.8R	specific target organ toxicity - single exposure (respiratory tract irritation)	3	STOT SE 3	H335

For full text of abbreviations: see SECTION 16.

2.2 **Label elements**

Labelling

- Signal word warning

- Pictograms

GHS07



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- Hazard statements

H315 Causes skin irritation.
 H319 Causes serious eye irritation.
 H335 May cause respiratory irritation.

- Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protec-

tion.

P312 Call a POISON CENTRE/doctor if you feel unwell.

P321 Specific treatment (see on this label).

P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P501 Dispose of contents/container to industrial combustion plant.

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) in a concentration of $\geq 0.1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Calconcarboxylic acid, Practical grade

Identifiers

CAS No 3737-95-9 EC No 223-117-0 Molecular formula $C_{21}H_{14}N_2O_7S$ Molar mass 438.41 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures

General notes

Do not leave affected person unattended. Remove victim out of the danger area. Keep affected person warm, still and covered. Take off immediately all contaminated clothing. In all cases of doubt, or when symptoms persist, seek medical advice. In case of unconsciousness place person in the recovery position. Never give anything by mouth.

Following inhalation

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions. In case of respiratory tract irritation, consult a physician. Provide fresh air.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Remove contact lenses, if present and easy to do. Continue rinsing. Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart.

Following ingestion

Rinse mouth with water (only if the person is conscious). Do NOT induce vomiting.

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4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Foam, ABC-powder

Unsuitable extinguishing media

Water jet

5.2 Special hazards arising from the substance or mixture

Deposited combustible dust has considerable explosion potential.

Hazardous combustion products

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. Co-ordinate firefighting measures to the fire surroundings. Do not allow firefighting water to enter drains or water courses. Collect contaminated firefighting water separately. Fight fire with normal precautions from a reasonable distance.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Remove persons to safety.

For emergency responders

Wear breathing apparatus if exposed to vapours/dust/spray/gases.

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.

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.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Recommendations

- Measures to prevent fire as well as aerosol and dust generation

Use local and general ventilation. Take precautionary measures against static discharge. Use only in well-ventilated areas. Ground/bond container and receiving equipment.

- Specific notes/details

Dust deposits may accumulate on all deposition surfaces in a technical room. The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

Advice on general occupational hygiene

Wash hands after use. Do not eat, drink and smoke in work areas. Remove contaminated clothing and protective equipment before entering eating areas. Never keep food or drink in the vicinity of chemicals. Never place chemicals in containers that are normally used for food or drink. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Managing of associated risks

- Explosive atmospheres

Removal of dust deposits.

- Ventilation requirements

Use local and general ventilation.

- Specific designs for storage rooms or vessels
- Storage temperature

Recommended storage temperature: 10 – 30 °C

7.3 Specific end use(s)

See section 16 for a general overview.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limit values (Workplace Exposure Limits)

Coun- try	Name of agent	CAS No	Identi- fier	TWA [mg/m³]	STEL [ppm]		Ceiling-C [mg/m³]		Source
GB	dust		WEL	10				i	EH40/ 2005
GB	dust		WEL	4				r	EH40/ 2005

Notation

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

i inhalable fraction r respirable fraction

STEL short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute peri-

od (unless otherwise specified)

TWA 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)

8.2 Exposure controls

Appropriate engineering controls

General ventilation.

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Individual protection measures (personal protective equipment)

Eye/face protection

Wear eye/face protection.

Skin protection

- Hand protection

Wear protective gloves.

- Other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended. Wash hands thoroughly after handling.

Respiratory protection

Particulate filter device (EN 143).

Environmental exposure controls

Use appropriate container to avoid environmental contamination. 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
Colour	Dark purple to black powder
Odour	characteristic
Melting point/freezing point	not determined
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)	not determined

Partition coefficient

Partition coefficient n-octanol/water (log value)	this information is not available
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Vapour pressure	not determined
Density and/or relative density	
Density	not determined
Relative vapour density	information on this property is not available
Particle characteristics	no data available
Other information	
Information with regard to physical hazard classes	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics	
Solid content	100 %

SECTION 10: Stability and reactivity

10.1 Reactivity

9.2

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials".

10.2 Chemical stability

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

No known hazardous reactions.

10.4 Conditions to avoid

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

Hints to prevent fire or explosion

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

10.5 Incompatible materials

Oxidisers

10.6 Hazardous decomposition products

Reasonably anticipated hazardous decomposition products produced as a result of use, storage, spill and heating are not known. Hazardous combustion products: see section 5.

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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 skin irritation.

Serious eye damage/eye irritation

Causes serious eye irritation.

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

May cause respiratory irritation.

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.

11.2 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

Data are not available.

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

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

12.6 Endocrine disrupting properties

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

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12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

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

Remarks

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

SECTION 14: Transport information

14.1	UN number or ID number	not subject to transport regulations

14.2 UN proper shipping name not relevant

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.

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)

Deco-Paint Directive

VOC content

VOC content	0 %			
Industrial Emissions Directive (IED)				

0 %

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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)

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

National inventories

Country	Inventory	Status
US	TSCA	substance is listed (ACTIVE)

Legend

TSCA

Toxic Substance Control Act

15.2 Chemical safety assessment

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

SECTION 16: Other information

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 identifier 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-li- cence/)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)

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Abbr.	Descriptions of used abbreviations
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
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
ppm	Parts per million
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)
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
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.

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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