

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



Neutron®Pharmaceutical Co.
Manufacturer of Laboratory Chemical & Pharmaceutical Materials

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Benzoic acid ROTI®CALIPURE Melting point standard 121-123 °C

article number: **1.1640**

Version: **2.0 en**

Replaces version of: 2015-08-28

Version: (1)

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

1.1 Product identifier

Identification of the substance	Benzoic acid
Article number	1.1640
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a)
Index No	607-705-00-8
EC number	200-618-2
CAS number	65-85-0

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

Identified uses:	laboratory chemical laboratory and analytical use
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1.3 Details of the supplier of the safety data sheet

98, 9th Floor, Borjsaz
Building, Azadi Ave,
Tehran, Iran.

Telephone: +98 (0)21-66906732

Telefax: +98 (0)21-66581408

e-mail: info@neutronpharmaceutical.com

Website: www.neutronpharmaceutical.com

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	

Emergency information service

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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.2	skin corrosion/irritation	(Skin Irrit. 2)	H315
3.3	serious eye damage/eye irritation	(Eye Dam. 1)	H318
3.9	specific target organ toxicity - repeated exposure	(STOT RE 1)	H372

2.2 Label elements

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

Signal word

Danger

Pictograms

GHS05, GHS08



Hazard statements

H315 Causes skin irritation
H318 Causes serious eye damage
H372 Causes damage to organs (lung) through prolonged or repeated exposure (if inhaled)

Precautionary statements

Precautionary statements - prevention

P260 Do not breathe dust.
P280 Wear protective gloves/eye protection.

Precautionary statements - response

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

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H318 Causes serious eye damage.
H372 Causes damage to organs (lung) through prolonged or repeated exposure (if inhaled).
P260 Do not breathe dust.
P280 Wear protective gloves/eye protection.
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.

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2.3 Other hazards

There is no additional information.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Phenylformic acid
Index No	607-705-00-8
EC number	200-618-2
CAS number	65-85-0
Molecular formula	C ₇ H ₆ O ₂
Molar mass	122,1 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Of Dust: Provide fresh air. In case of respiratory tract irritation, consult a physician.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

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.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Irritation, Cough, Headache, Gastrointestinal complaints, Nausea, Vomiting, Diarrhoea, Dyspnoea, Risk of serious damage to eyes

4.3 Indication of any immediate medical attention and special treatment needed

none

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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

Hazardous combustion products

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

5.3 Advice for firefighters

Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

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.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

Advices 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

7.1 Precautions for safe handling

Provide adequate ventilation. 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

Keep container tightly closed. 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.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Country	Name of agent	CAS No	Notation	Identifier	TWA [mg/m ³]	STEL [mg/m ³]	Source
GB	dust		i	WEL	10		EH40/2005
GB	dust		r	WEL	4		EH40/2005

Notation

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 period (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)

Relevant DNELs/DMELs/PNECs and other threshold levels

• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	3 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	0,1 mg/m ³	human, inhalatory	worker (industry)	chronic - local effects
DNEL	62,5 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

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• environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	0,331 mg/l	water	intermittent release
PNEC	0,34 mg/l	freshwater	short-term (single instance)
PNEC	0,034 mg/l	marine water	short-term (single instance)
PNEC	100 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	1,75 mg/kg	freshwater sediment	short-term (single instance)
PNEC	0,175 mg/kg	marine sediment	short-term (single instance)
PNEC	0,151 mg/kg	soil	short-term (single instance)

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.

• 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). P2 (filters at least 94 % of airborne particles, colour code: White).

Environmental exposure controls

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Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	solid (powder)
Colour	white
Odour	odourless
Odour threshold	No data available

Other physical and chemical parameters

pH (value)	2,5 – 3,5 (20 °C) (aqueous solution of the substance)
Melting point/freezing point	122,4 °C
Initial boiling point and boiling range	249 °C at 1.013 hPa
Flash point	121 °C (c.c.)
Evaporation rate	no data available
Flammability (solid, gas)	These information are not available
<u>Explosive limits</u>	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	these information are not available
Vapour pressure	0,001 hPa at 20 °C
Density	1,321 g/cm ³ at 20 °C
Vapour density	This information is not available.
Bulk density	~ 500 kg/m ³
Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	3,5 g/l at 25 °C
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	1,88 (ECHA)
Soil organic carbon/water (log KOC)	1,191 (ECHA)
Auto-ignition temperature	570 °C
Decomposition temperature	no data available
Viscosity	not relevant (solid matter)
Explosive properties	Shall not be classified as explosive
Oxidising properties	none

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9.2 Other information

Surface tension

67,5 ^{mN} /m (20 °C)

Temperature class (EU, acc. to ATEX)

T1 (Maximum permissible surface temperature on the equipment: 450°C)

SECTION 10: Stability and reactivity

10.1 Reactivity

Dust explosibility, If heated: Vapours can form explosive mixtures with air

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: Alkalis, Fluorine, Reducing agents, Oxygen, Strong oxidiser

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

Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
oral	LD50	2.360 ^{mg} /kg	rat	ECHA
inhalation: dust/mist	LC50	>12.200 ^{mg} /m ³ /4h	rat	ECHA
dermal	LD50	>2.000 ^{mg} /kg	rabbit	ECHA

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/eye irritation

Causes serious eye damage.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor 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

Causes damage to organs (lung) through prolonged or repeated exposure (if inhaled).

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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

gastrointestinal complaints, nausea, vomiting, diarrhoea

• If in eyes

Causes serious eye damage, risk of blindness

• If inhaled

irritant effects, cough, headache, breathing difficulties, varying degrees of pulmonary injury

• If on skin

causes skin irritation

Other information

None.

SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
EC50	252 ^{mg} / _l	Tetrahymena pyriformis	ECOTOX Database	48 h
LC50	44,6 ^{mg} / _l	bluegill	ECHA	96 h
ErC50	>33,1 ^{mg} / _l	algae	ECHA	72 h

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
EC50	>120 ^{mg} / _l	rainbow trout (Oncorhynchus mykiss)	ECHA	28 d
EC50	>25 ^{mg} / _l	daphnia magna	ECHA	21 d
NOEC	>120 ^{mg} / _l	rainbow trout (Oncorhynchus mykiss)	ECHA	28 d
NOEC	≥25 ^{mg} / _l	daphnia magna	ECHA	21 d

12.2 Process of degradability

The substance is readily biodegradable.

Theoretical Oxygen Demand: 1,965 ^{mg}/_{mg}

Theoretical Carbon Dioxide: 2,523 ^{mg}/_{mg}

Process	Degradation rate	Time
biotic/abiotic	>70 %	5 d
carbon dioxide generation	89,5 %	35 d

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12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW) 1,88

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient 1,191

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 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.

Sewage disposal-relevant information

Do not empty into drains.

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.

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.

SECTION 14: Transport information

- | | | |
|------|--|--|
| 14.1 | UN number | (not subject to transport regulations) |
| 14.2 | UN proper shipping name | not relevant |
| 14.3 | Transport hazard class(es) | not relevant |
| | Class | - |
| 14.4 | Packing group | not relevant not assigned to a packing group |
| 14.5 | Environmental hazards | none (non-environmentally hazardous acc. to the dangerous goods regulations) |
| 14.6 | Special precautions for user | |
| | There is no additional information. | |
| 14.7 | Transport in bulk according to Annex II of MARPOL and the IBC Code | |
| | The cargo is not intended to be carried in bulk. | |

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14.8 Information for each of the UN Model Regulations

- **Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)**

Not subject to ADR, RID and ADN.

- **International Maritime Dangerous Goods Code (IMDG)**

Not subject to IMDG.

- **International Civil Aviation Organization (ICAO-IATA/DGR)**

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)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**

Not listed.

- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

- **Restrictions according to REACH, Annex XVII**

not listed

- **Restrictions according to REACH, Title VIII**

None.

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

not listed

- **Directive 75/324/EEC relating to aerosol dispensers**

Filling batch

Deco-Paint Directive (2004/42/EC)

VOC content	100 % 1.321 g/l
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Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

Regulation 98/2013/EU on the marketing and use of explosives precursors

not listed

Regulation 111/2005/EC laying down rules for the monitoring of trade between the Community and third countries in drug precursors

not listed

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National inventories

Substance is listed in the following national inventories:

Country	National inventories	Status
AU	AICS	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

AICS	Australian Inventory of Chemical Substances
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
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
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DGR	Dangerous Goods Regulations (see IATA/DGR)

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Abbr.	Descriptions of used abbreviations
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
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
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
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
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
SVHC	Substance of Very High Concern
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

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

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

Code	Text
H315	causes skin irritation
H318	causes serious eye damage
H372	causes damage to organs (lung) through prolonged or repeated exposure (if inhaled)

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Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.