

1 Identification

Product identifier

Product name: 4-Hydroxy-3,5-diiodobenzonitrile

Stock number: L05423

CAS Number:
1689-83-4

EC number:
216-881-1

Index number:
608-007-00-6

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

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757
Email: tech@alfa.com
www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS06 Skull and crossbones

Acute Tox. 3 H301 Toxic if swallowed.

Acute Tox. 3 H331 Toxic if inhaled.



GHS08 Health hazard

Repr. 2 H361 Suspected of damaging fertility or the unborn child.

STOT RE 2 H373 May cause damage to the lung, the liver and the endocrine system through prolonged or repeated exposure. Route of exposure: Oral.



GHS07

Acute Tox. 4 H312 Harmful in contact with skin.

Eye Irrit. 2 H319 Causes serious eye irritation.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS06 GHS08

Signal word

Danger

Hazard statements

H301+H331 Toxic if swallowed or if inhaled.

H312 Harmful in contact with skin.

H319 Causes serious eye irritation.

H361 Suspected of damaging fertility or the unborn child.

H373 May cause damage to the lung, the liver and the endocrine system through prolonged or repeated exposure. Route of exposure: Oral.

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

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

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...

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

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

D1A - Very toxic material causing immediate and serious toxic effects

D2A - Very toxic material causing other toxic effects



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 2 Health (acute effects) = 2

FIRE 1 Flammability = 1

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

Product name: 4-Hydroxy-3,5-diiodobenzonitrile

vPvB: Not applicable.

(Contd. of page 1)

3 Composition/information on ingredients

Chemical characterization: Substances
CAS# Description:
1689-83-4 4-Hydroxy-3,5-diiodobenzonitrile
Identification number(s):
EC number: 216-881-1
Index number: 608-007-00-6

4 First-aid measures

Description of first aid measures
General information
Immediately remove any clothing soiled by the product.
Remove breathing apparatus only after contaminated clothing has been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Do not induce vomiting; immediately call for medical help.
Information for doctor
Most important symptoms and effects, both acute and delayed No further relevant information available.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media
Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
Special hazards arising from the substance or mixture
If this product is involved in a fire, the following can be released:
Carbon monoxide and carbon dioxide
Nitrogen oxides (NOx)
Hydrogen iodide (HI)
Hydrogen cyanide (HCN)
Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Environmental precautions: Do not allow material to be released to the environment without proper governmental permits.
Methods and material for containment and cleaning up:
Dispose of contaminated material as waste according to section 13.
Ensure adequate ventilation.
Prevention of secondary hazards: No special measures required.
Reference to other sections
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage

Handling
Precautions for safe handling
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Open and handle container with care.
Information about protection against explosions and fires: No information known.
Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: No special requirements.
Information about storage in one common storage facility:
Store away from oxidizing agents.
Store in the dark.
Further information about storage conditions:
Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.
Protect from exposure to light.
Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.
Control parameters
Components with limit values that require monitoring at the workplace: Not required.
Additional information: No data
Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.

(Contd. on page 3)

Product name: 4-Hydroxy-3,5-diiodobenzonitrile

(Contd. of page 2)

Wash hands before breaks and at the end of work.
Store protective clothing separately.
Avoid contact with the eyes.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.
Breathing equipment: Use self-contained respiratory protective device in emergency situations.
Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.
Penetration time of glove material (in minutes) Not determined
Eye protection: Safety glasses
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form: Powder
Color: White
Odor: Odorless
Odor threshold: Not determined.

pH-value: Not applicable.

Change in condition

Melting point/Melting range: 200-207 °C (392-405 °F)
Boiling point/Boiling range: Not determined
Sublimation temperature / start: Not determined
Flammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined.

Danger of explosion: Product does not present an explosion hazard.

Explosion limits:

Lower: Not determined
Upper: Not determined
Vapor pressure at 20 °C (68 °F): <0.00001 hPa (<0 mm Hg)
Density: Not determined
Relative density Not determined.
Vapor density Not applicable.
Evaporation rate Not applicable.

Solubility in / Miscibility with

Water at 20 °C (68 °F): 0.05-0.1 g/l
Partition coefficient (n-octanol/water): Not determined.
Viscosity:
dynamic: Not applicable.
kinematic: Not applicable.
Other information No further relevant information available.

10 Stability and reactivity

Reactivity No information known.

Chemical stability Stable under recommended storage conditions.

Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.

Possibility of hazardous reactions No dangerous reactions known

Conditions to avoid No further relevant information available.

Incompatible materials:

Oxidizing agents
Light

Hazardous decomposition products:

Carbon monoxide and carbon dioxide
Nitrogen oxides
Hydrogen iodide (HI)
Hydrogen cyanide

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful in contact with skin.
Toxic if inhaled.
Toxic if swallowed.
Danger through skin absorption.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for components in this product.

LD/LC50 values that are relevant for classification:

Oral	LD50	110 mg/kg (rat)
Inhalative	LC50/4H	0.38 mg/l/4H (rat)

Skin irritation or corrosion: May cause irritation

Eye irritation or corrosion: Causes serious eye irritation.

Sensitization: No sensitizing effects known.

Germ cell mutagenicity: No effects known.

Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

Reproductive toxicity: Suspected of damaging fertility or the unborn child.

Specific target organ system toxicity - repeated exposure:

May cause damage to the lung, the liver and the endocrine system through prolonged or repeated exposure. Route of exposure: Oral.

Specific target organ system toxicity - single exposure: No effects known.

Aspiration hazard: No effects known.

Subacute to chronic toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for this substance.

Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

Product name: 4-Hydroxy-3,5-diiodobenzonitrile

(Contd. of page 3)




12 Ecological information

Toxicity
Aquatic toxicity: No further relevant information available.
Persistence and degradability No further relevant information available.
Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Ecotoxicological effects:
Remark: Very toxic for aquatic organisms
Additional ecological information:
General notes:
Do not allow material to be released to the environment without proper governmental permits.
Do not allow product to reach ground water, water course or sewage system, even in small quantities.
Danger to drinking water if even extremely small quantities leak into the ground.
Also poisonous for fish and plankton in water bodies.
May cause long lasting harmful effects to aquatic life.
Avoid transfer into the environment.
Very toxic for aquatic organisms
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.



13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, IMDG, IATA	UN3439
UN proper shipping name DOT IMDG IATA	Nitriles, solid, toxic, n.o.s. (4-Hydroxy-3,5-diiodobenzonitrile) NITRILES, SOLID, TOXIC, N.O.S. (4-Hydroxy-3,5-diiodobenzonitrile), MARINE POLLUTANT NITRILES, SOLID, TOXIC, N.O.S. (4-Hydroxy-3,5-diiodobenzonitrile)
Transport hazard class(es) DOT  Class Label Class Label IMDG  Class Label IATA  Class Label	6.1 Toxic substances. 6.1 6.1 (T2) Toxic substances 6.1 6.1 Toxic substances. 6.1 6.1 Toxic substances. 6.1
Packing group DOT, IMDG, IATA	III
Environmental hazards: Marine pollutant (IMDG):	Environmentally hazardous substance, solid; Marine Pollutant Symbol (fish and tree)
Special precautions for user	Warning: Toxic substances
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information: DOT Marine Pollutant (DOT): Remarks:	No Special marking with the symbol (fish and tree).
UN "Model Regulation":	UN3439, Nitriles, solid, toxic, n.o.s. (4-Hydroxy-3,5-diiodobenzonitrile), 6.1, III

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms


GHS06 GHS08
Signal word Danger
Hazard statements
H301+H331 Toxic if swallowed or if inhaled.

Product name: 4-Hydroxy-3,5-diiodobenzonitrile

(Contd. of page 4)

H312 Harmful in contact with skin.
H319 Causes serious eye irritation.
H361 Suspected of damaging fertility or the unborn child.
H373 May cause damage to the lung, the liver and the endocrine system through prolonged or repeated exposure. Route of exposure: Oral.

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor/...
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

National regulations

This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.

SARA Section 313 (specific toxic chemical listings) Substance is not listed.

California Proposition 65

Prop 65 - Chemicals known to cause cancer Substance is not listed.

Prop 65 - Developmental toxicity Substance is not listed.

Prop 65 - Developmental toxicity, female Substance is not listed.

Prop 65 - Developmental toxicity, male Substance is not listed.

Information about limitation of use: For use only by technically qualified individuals.

Other regulations, limitations and prohibitive regulations

Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.

The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.

Substance is not listed.

Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.

Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department

Date of preparation / last revision 11/23/2015 / -

Abbreviations and acronyms:

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
ICAO: International Civil Aviation Organization
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)