

2-FLUORO-4-HYDROXYBENZONITRILE

Page: 1

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# Section 1: Identification of the substance/mixture and of the company/undertaking

## 1.1. Product identifier

Product name: 2-FLUORO-4-HYDROXYBENZONITRILE

CAS number: 82380-18-5

EINECS number: 422-810-7

Index number: 608-062-00-6

Product code: PC0409

Synonyms: 4-CYANO-3-FLUOROPHENOL

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

# 1.3. Details of the supplier of the safety data sheet

Company name: Apollo Scientific Ltd Units 3 & 4 Parkway Denton Manchester M34 3SG UK Tel: 0161 337 9971 Fax: 0161 336 6932 Email: david.tideswell@apolloscientific.co.uk

## 1.4. Emergency telephone number

# Section 2: Hazards identification

2.1. Classification of the substance or mixture		
Classification under CHIP:	Xn: R22; Xi: R41; N: R51/53	
Classification under CLP:	Acute Tox. 4: H302; Eye Dam. 1: H318; Aquatic Chronic 2: H411	
Most important adverse effects: Harmful if swallowed. Risk of serious damage to eyes. Toxic to aquatic organisms, may		
	cause long-term adverse effects in the aquatic environment.	
2.2. Label elements		
Label elements under CLP:		
Hazard statements:	H302: Harmful if swallowed.	
	H318: Causes serious eye damage.	
	H411: Toxic to aquatic life with long lasting effects.	
Signal words:	Danger	

## 2-FLUORO-4-HYDROXYBENZONITRILE

Hazard pictograms: GHS09: Environmental GHS05: Corrosion GHS07: Exclamation mark Precautionary statements: P280: Wear protective gloves/protective clothing/eye protection/face protection. P309+311: IF exposed or if you feel unwell: Call a POISON CENTER or doctor. Label elements under CHIP: Hazard symbols: Dangerous for the environment. Harmful. Risk phrases: R22: Harmful if swallowed. R41: Risk of serious damage to eyes. R51/53: Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. Safety phrases: S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S36/37/39: Wear suitable protective clothing, gloves and eye / face protection. 2.3. Other hazards **PBT:** This substance is not identified as a PBT substance.

# Section 3: Composition/information on ingredients

# 3.1. Substances

Chemical identity: 2-FLUORO-4-HYDROXYBENZONITRILE

# Section 4: First aid measures

# 4.1. Description of first aid measures

Skin contact:	Remove all contaminated clothes and footwear immediately unless stuck to skin.	
	Drench the affected skin with running water for 10 minutes or longer if substance is still	
	on skin. Consult a doctor.	
Eye contact:	Bathe the eye with running water for 15 minutes. Consult a doctor.	
Ingestion:	: Wash out mouth with water. Do not induce vomiting. If conscious, give half a litre of water	
	to drink immediately. Consult a doctor.	

Inhalation: Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a doctor.

# Page: 2

#### 2-FLUORO-4-HYDROXYBENZONITRILE

#### 4.2. Most important symptoms and effects, both acute and delayed

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

**Ingestion:** There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

**Inhalation:** There may be irritation of the throat with a feeling of tightness in the chest.

## 4.3. Indication of any immediate medical attention and special treatment needed

#### Section 5: Fire-fighting measures

## 5.1. Extinguishing media

**Extinguishing media:** Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the surrounding fire should be used. Use water spray to cool containers.

#### 5.2. Special hazards arising from the substance or mixture

**Exposure hazards:** In combustion emits toxic fumes. Carbon oxides. Nitrogen oxides (NOx). Hydrogen fluoride (HF).

#### 5.3. Advice for fire-fighters

Advice for fire-fighters: Wear self-contained breathing apparatus. Wear protective clothing to prevent contact with skin and eyes.

## Section 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

**Personal precautions:** Refer to section 8 of SDS for personal protection details. If outside do not approach from downwind. If outside keep bystanders upwind and away from danger point. Mark out the contaminated area with signs and prevent access to unauthorised personnel.

6.2. Environmental precautions

Environmental precautions: Do not discharge into drains or rivers.

#### 6.3. Methods and material for containment and cleaning up

Clean-up procedures: Transfer to a closable, labelled salvage container for disposal by an appropriate

method.

## 6.4. Reference to other sections

#### Section 7: Handling and storage

#### 7.1. Precautions for safe handling

Handling requirements: Avoid direct contact with the substance. Ensure there is sufficient ventilation of the area. Do not handle in a confined space. Avoid the formation or spread of dust in the air. Only use in fume hood.

# 2-FLUORO-4-HYDROXYBENZONITRILE

		Page:	4
7.2. Conditions for safe storage, including any incompatibilities			
Storage conditions:	Store in cool, well ventilated area. Keep container tightly closed. The floor of the storage		
	room must be impermeable to prevent the escape of liquids. Store under Argon.		
Suitable packaging:	Must only be kept in original packaging.		
7.3. Specific end use(s)			
Specific end use(s):	No data available.		
Section 8: Exposure controls/personal protection			
8.1. Control parameters			
	Net employed		
Workplace exposure limits:			_
8.2. Exposure controls			
Engineering measures:	Ensure there is sufficient ventilation of the area. The floor of the storage room must be		
	impermeable to prevent the escape of liquids.		
Respiratory protection:	Self-contained breathing apparatus must be available in case of emergency. Respiratory		
	protective device with particle filter.		
Hand protection:	Protective gloves.		
Eye protection:	Safety glasses. Ensure eye bath is to hand.		
Skin protection:	Protective clothing.		
Section 9: Physical and chemi	cal properties		
9.1. Information on basic physic	ical and chemical properties		
and mation on basic physic			
State:	Solid		
Colour:	White		
Oxidising:	Non-oxidising (by EC criteria)		
	A00 400		

Melting point/range °C: 123-126

**pH:** 4.2

Relative density: 1.45

9.2. Other information

Other information: Not applicable.

# Section 10: Stability and reactivity

10.1. Reactivity

**Reactivity:** Stable under recommended transport or storage conditions.

10.2. Chemical stability

Chemical stability: Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous reactions: Hazardous reactions will not occur under normal transport or storage conditions.

## 2-FLUORO-4-HYDROXYBENZONITRILE

### 10.4. Conditions to avoid

# Conditions to avoid: Heat.

## 10.5. Incompatible materials

Materials to avoid: Strong oxidising agents. Strong acids.

# 10.6. Hazardous decomposition products

Haz. decomp. products: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides

(NOx). Hydrogen fluoride (HF).

## Section 11: Toxicological information

#### 11.1. Information on toxicological effects

## **Toxicity values:**

Route	Species	Test	Value	Units
ORAL	RAT	LD50	688	mg/kg

#### Relevant hazards for substance:

Hazard	Route	Basis
Acute toxicity (ac. tox. 4)	ING	Based on test data
Serious eye damage/irritation	OPT	Based on test data

## Symptoms / routes of exposure

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach

pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

## Section 12: Ecological information

#### 12.1. Toxicity

Ecotoxicity values: Not applicable.

#### 12.2. Persistence and degradability

Persistence and degradability: No data available.

12.3. Bioaccumulative potential

Bioaccumulative potential: No data available.

12.4. Mobility in soil

Mobility: No data available.

## 2-FLUORO-4-HYDROXYBENZONITRILE

Page: 6

#### 12.5. Results of PBT and vPvB assessment

PBT identification: This substance is not identified as a PBT substance.

# 12.6. Other adverse effects

Other adverse effects: Toxic to aquatic organisms.

#### Section 13: Disposal considerations

13.1. Waste treatment methods

# **Disposal operations:** MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL, STATE AND FEDERAL REGULATIONS

**Disposal of packaging:** Dispose of as special waste in compliance with local and national regulations Observe all federal, state and local environmental regulations.

**NB:** The user's attention is drawn to the possible existence of regional or national regulations regarding disposal.

Section 14: Transport information

14.1. UN number

UN number: UN3077

14.2. UN proper shipping name

Shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

14.3. Transport hazard class(es)

Transport class: 9

14.4. Packing group

Packing group: III

14.5. Environmental hazards

Environmentally hazardous: Yes

14.6. Special precautions for user

Marine pollutant: No

Tunnel code: E

Transport category: 3

# Section 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

# 15.2. Chemical Safety Assessment

Chemical safety assessment: A chemical safety assessment has not been carried out for the substance or the mixture

by the supplier.

# Section 16: Other information

# 2-FLUORO-4-HYDROXYBENZONITRILE

Other information	
Other information:	This safety data sheet is prepared in accordance with Commission Regulation (EU) No 453/2010.
	* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by
	decision tree approach. http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?
	c=TOXTREE
	~ Data predicted using computatioanl software ACD/ToxSuite v 2.95.1 Copyright 1994-
	2009 ACD/labs, Copyright 2001-2009 Pharma Algorithms, Inc, Advanced Chemistry
	Development, Inc (ACD/Labs). http://www.acdlabs.com/products/pc_admet/tox/tox/
Phrases used in s.2 and 3:	H302: Harmful if swallowed.
	H318: Causes serious eye damage.
	H411: Toxic to aquatic life with long lasting effects.
	R22: Harmful if swallowed.
	R41: Risk of serious damage to eyes.
	R51/53: Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic
	environment.
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