

SAFETY DATA SHEET
3-CHLORO-4-METHYLBENZONITRILE

Page: 1
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Revision No: 3

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

1.1. Product identifier

Product name: 3-CHLORO-4-METHYLBENZONITRILE
CAS number: 21423-81-4
EINECS number: * 244-381-3
Product code: OR3687
Synonyms: * 3-CHLORO-P-TOLUNITRILE
2-CHLORO-4-CYANOTOLUENE

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 CLP: STOT SE 3: H335; Eye Irrit. 2: H319; Flam. Sol. 1: H228; Skin Irrit. 2: H315

Classification under CHIP: F: R11; Xi: R36/37/38

Most important adverse effects: Flammable solid. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

2.2. Label elements

Label elements:

Hazard statements: H228: Flammable solid.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H335: May cause respiratory irritation.

SAFETY DATA SHEET
3-CHLORO-4-METHYLBENZONITRILE

Page: 2

Signal words: Danger

Hazard pictograms: GHS02: Flame

GHS07: Exclamation mark



Precautionary statements: P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P260: Do not breathe dust.

P280: Wear protective gloves/protective clothing/eye protection/face protection.

2.3. Other hazards

PBT: This product is not identified as a PBT/vPvB substance.

Section 3: Composition/information on ingredients

3.1. Substances

Chemical identity: 3-CHLORO-4-METHYLBENZONITRILE

CAS number: 21423-81-4

EINECS number: * 244-381-3

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. Wash immediately with plenty of soap and water.

Eye contact: Bathe the eye with running water for 15 minutes. Consult a doctor.

Ingestion: Wash out mouth with water. Consult a doctor.

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

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.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest. Exposure may cause coughing or wheezing.

Delayed / immediate effects: No data available.

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

Immediate / special treatment: No data available.

Section 5: Fire-fighting measures

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SAFETY DATA SHEET
3-CHLORO-4-METHYLBENZONITRILE

Page: 3

5.1. Extinguishing media

Extinguishing media: Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the surrounding fire should be used.

5.2. Special hazards arising from the substance or mixture

Exposure hazards: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NO_x). Hydrogen chloride (HCl). Hydrogen cyanide (HCN).

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. Do not create dust.

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

Reference to other sections: Refer to section 8 of SDS.

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.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions: Store in a cool, well ventilated area. Keep container tightly closed.

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

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SAFETY DATA SHEET
3-CHLORO-4-METHYLBENZONITRILE

Page: 4

8.1. Control parameters

Workplace exposure limits: No data available.

DNEL/PNEC Values

DNEL / PNEC No data available.

8.2. Exposure controls

Engineering measures: Ensure there is sufficient ventilation of the area.

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.

Environmental: Not applicable.

Section 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

State: Powder

Colour: White

Oxidising: Non-oxidising (by EC criteria)

Melting point/range °C: 45-48

Flash point °C: 84

9.2. Other information

Other information: No data available.

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.

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 cyanide (HCN). Hydrogen chloride (HCl).

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SAFETY DATA SHEET
3-CHLORO-4-METHYLBENZONITRILE

Page: 5

Section 11: Toxicological information

11.1. Information on toxicological effects

Relevant hazards for substance:

Hazard	Route	Basis
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data
STOT-single exposure	INH	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.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest. Exposure may cause coughing or wheezing.

Delayed / immediate effects: No data available.

Other information: Not applicable.

Section 12: Ecological information

12.1. Toxicity

Ecotoxicity values: No data available.

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.

12.5. Results of PBT and vPvB assessment

PBT identification: This product is not identified as a PBT/vPvB substance.

12.6. Other adverse effects

Other adverse effects: No data available.

Section 13: Disposal considerations

13.1. Waste treatment methods

Disposal operations: Transfer to a suitable container and arrange for collection by specialised disposal company. 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.

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SAFETY DATA SHEET
3-CHLORO-4-METHYLBENZONITRILE

Page: 6

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: UN1325

14.2. UN proper shipping name

Shipping name: FLAMMABLE SOLID, ORGANIC, N.O.S.
(3-Chloro-4-methylbenzotrile)

14.3. Transport hazard class(es)

Transport class: 4.1

14.4. Packing group

Packing group: II

14.5. Environmental hazards

Environmentally hazardous: No

Marine pollutant: No

14.6. Special precautions for user

Tunnel code: E

Transport category: 2

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

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 computational 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 s.3: H228: Flammable solid.

H315: Causes skin irritation.

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SAFETY DATA SHEET

3-CHLORO-4-METHYLBENZONITRILE

Page: 7

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

R11: Highly flammable.

R36/37/38: Irritating to eyes, respiratory system and skin.

Legend to abbreviations: PNEC = predicted no effect level
DNEL = derived no effect level
LD50 = median lethal dose
LC50 = median lethal concentration
EC50 = median effective concentration
IC50 = median inhibitory concentration
dw = dry weight
bw = body weight
cc = closed cup
oc = open cup
MUS = mouse
GPG = guinea pig
RBT = rabbit
HAM = hamster
HMN = human
MAM = mammal
PGN = pigeon
IVN = intravenous
SCU = subcutaneous
SKN = skin
DRM = dermal
OCC = ocular/corneal
PCP = physico-chemical properties

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