

Chemical Safety Data Sheet MSDS / SDS

TRANS-4-(5-PENTYL-1,3-DIOXAN-2-YL)BENZONITRILE

Revision Date:2026-05-31 Revision Number:1

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

Product name : TRANS-4-(5-PENTYL-1,3-DIOXAN-2-YL)BENZONITRILE
CBnumber : CB4130248
CAS : 74800-62-7
EINECS Number : 278-001-2
Synonyms : PDX-5;LABOTEST-BB LT00080429

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P405 Store locked up.

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

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

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

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

Hazard statements

H302 Harmful if swallowed

H312 Harmful in contact with skin

H315 Causes skin irritation

H319 Causes serious eye irritation

H331 Toxic if inhaled

H335 May cause respiratory irritation

SECTION 3: Composition/information on ingredients

Substance

Product name : TRANS-4-(5-PENTYL-1,3-DIOXAN-2-YL)BENZONITRILE
Synonyms : PDX-5;LABOTEST-BB LT00080429
CAS : 74800-62-7
EC number : 278-001-2
MF : C16H21NO2
MW : 259.34

SECTION 4: First aid measures

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

Most important symptoms and ef

None reasonably foreseeable.

Self-Protection of the First Aider

No special precautions required.

Notes to Physician

Treat symptomatically.

SECTION 5: Firefighting measures

Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Extinguishing media which must not be used for safety reasons

No information available.

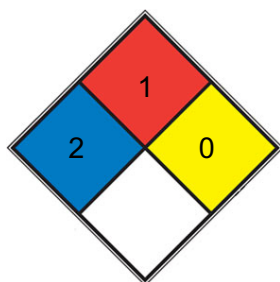
Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

SPEC.
 HAZ.

SECTION 6: Accidental release measures

Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: Handling and storage

Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid ingestion and inhalation. Avoid dust formation. Do not get in eyes, on skin, or on clothing.

Storage

Store under an inert atmosphere.

Specific Use(s)

Use in laboratories

SECTION 8: Exposure controls/personal protection

Control Parameters

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

Exposure Controls

Engineering Measures

None under normal use conditions. Ensure that eyewash stations and safety showers are close to the workstation location. .

Personal protective equipment

Eye Protection

Goggles (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g.

sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection

Long sleeved clothing

Respiratory Protection

No protective equipment is needed under normal use conditions.

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Particle filter

Small scale/Laboratory use

Maintain adequate ventilation

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls

No information available.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

No information available

Physical State

Solid

Odor

No information available

Odor Threshold

No data available

pH

No information available

Melting Point/Range

56 - 58 °C / 132.8 - 136.4 °F

Softening Point

No data available

Boiling Point/Range

393.0±37.0 °C(Predicted)

Flash Point

No information available

Method - No information available

Evaporation Rate

Not applicable Solid

Flammability (solid,gas)

No information available

Explosion Limits

No data available

Vapor Pressure

No data available

Vapor Density

Not applicable Solid

Specific Gravity / Density

1.07±0.1 g/cm³(Predicted)

Bulk Density

1.07±0.1 g/cm³(Predicted)

Water Solubility

No information available

Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

No data available

Autoignition Temperature

No data available

Decomposition Temperature

No data available

Viscosity

Not applicable Solid

Explosive Properties

No information available

Oxidizing Properties

No information available

SECTION 10: Stability and reactivity

Stability

Air sensitive.

Hazardous Reactions

None under normal processing.

Hazardous Polymerization

No information available.

Conditions to Avoid

None known.

Materials to avoid

No information available.

Hazardous Decomposition Products

None under normal use conditions.

SECTION 11: Toxicological information

Product Information

(a) acute toxicity;

(b) skin corrosion/irritation;

Category 2

(c) serious eye damage/irritation;

Category 2

(d) respiratory or skin sensitization;

Respiratory

No data available

Skin

No data available

(e) germ cell mutagenicity;

No data available

(f) carcinogenicity;

No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity;

No data available

(h) STOT-single exposure;

Category 3

Results / Target organs

Respiratory system

(i) STOT-repeated exposure;

No data available

Target Organs

No information available.

(j) aspiration hazard;

Not applicable

Solid

Symptoms / effects,both acute and delayed

No information available

SECTION 12: Ecological information

Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability

No information available

Bioaccumulative Potential

No information available

Mobility in soil

No information available

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

Persistent Organic Pollutant

This product does not contain any known or suspected substance

Ozone Depletion Potential

This product does not contain any known or suspected substance

SECTION 13: Disposal considerations

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14: Transport information

Road and Rail Transport

UN-No

UN3439

Proper Shipping Name

NITRILES, SOLID, TO XIC, N.O.S.

Technical Shipping Name

(2-(4-Cyanophenyl)-5- n-pentyl-1,3-dioxane)

Hazard Class

6.1

Packing Group

III

IMDG/IMO

UN-No

UN3439

Proper Shipping Name

NITRILES, SOLID, TO XIC, N.O.S.

Technical Shipping Name

(2-(4-Cyanophenyl)-5- n-pentyl-1,3-dioxane)

Hazard Class

6.1

Packing Group

III

IATA

UN-No

UN3439

Proper Shipping Name	NITRILES, SOLID, TOXIC, N.O.S.
Technical Shipping Name	(2-(4-Cyanophenyl)-5-n-pentyl-1,3-dioxane)

Hazard Class					6.1
Packing Group					III
Special Precautions for User	No special precautions required				

SECTION 15: Regulatory information

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
4-(5-Pentyl-1,3-dioxan-2-yl)benzotrile	-	-		X	278-001-2	-	-	-	-	-	-	-

National Regulations

SECTION 16: Other information

Prepared By

Health, Safety and Environmental Department

Revision Date

24-Sep-2025

Revision Summary

Not applicable.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Legend

CAS

Chemical Abstracts Service

TSCA

United States Toxic Substances Control Act Section 8(b)

Inventory

EINECS/ELINCS

European Inventory of Existing Commercial Chemical

Substances/EU List of Notified Chemical Substances

DSL/NDSL

Canadian Domestic Substances List/Non-Domestic

Substances List

PICCS

Philippines Inventory of Chemicals and Chemical Substances

ENCS

Japanese Existing and New Chemical Substances

IECSC

Chinese Inventory of Existing Chemical Substances

AICS

Australian Inventory of Chemical Substances

KECL

Korean Existing and Evaluated Chemical Substances

NZIoC

New Zealand Inventory of Chemicals

WEL

Workplace Exposure Limit

TWA

Time Weighted Average

ACGIH

American Conference of Governmental Industrial Hygienists

IARC

International Agency for Research on Cancer

DNEL

Derived No Effect Level

PNEC

Predicted No Effect Concentration

RPE

Respiratory Protective Equipment

LD50

Lethal Dose 50%

LC50

Lethal Concentration 50%

EC50

Effective Concentration 50%

NOEC

No Observed Effect Concentration

POW

Partition coefficient Octanol:Water

PBT

Persistent, Bioaccumulative, Toxic

vPvB

very Persistent, very Bioaccumulative

ICAO/IATA

International Civil Aviation Organization/International Air
Transport Association

IMO/IMDG

International Maritime Organization/International Maritime
Dangerous Goods Code

ADR

European Agreement Concerning the International Carriage of
Dangerous Goods by Road

MARPOL

International Convention for the Prevention of Pollution from
Ships

OECD

Organisation for Economic Co-operation and Development

ATE

Acute Toxicity Estimate

BCF

Bioconcentration factor

VOC

(Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.