

Creation Date 04-Aug-2015

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Revision Number 2

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identification

Product Description: **1-Phenyl-1-cyclopentanecarbonitrile**
 Cat No. : **136100000; 136100100; 136100500**
 CAS-No **77-57-6**
 EC-No. **201-038-2**
 Molecular Formula **C12 H13 N**

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

Recommended Use Laboratory chemicals.
 Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company Acros Organics BVBA
 Janssen Pharmaceuticaaan 3a
 2440 Geel, Belgium
 E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

Environmental hazards

Based on available data, the classification criteria are not met

2.2. Label elements

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Signal Word

Warning

Hazard Statements

H302 - Harmful if swallowed
H312 - Harmful in contact with skin
H315 - Causes skin irritation
H335 - May cause respiratory irritation
H319 - Causes serious eye irritation
H332 - Harmful if inhaled

Precautionary Statements

P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P312 - Call a POISON CENTER or doctor/ physician if you feel unwell
P304 + P340 - IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P261 - Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray

2.3. Other hazards

No information available

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008
1-Phenylcyclohexanecarbonitrile	77-57-6	EEC No. 201-038-2	>95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of 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.
Obtain medical attention.

Skin Contact

Obtain medical attention. Wash off immediately with plenty of water for at least 15 minutes.

Ingestion

Clean mouth with water and drink afterwards plenty of water.

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Inhalation Move to fresh air. If breathing is difficult, give oxygen. Obtain medical attention.

Protection of First-aiders Use personal protective equipment.

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

None reasonably foreseeable.

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

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

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

Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂).

5.3. Advice for firefighters

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

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Ensure adequate ventilation.

6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional ecological information.

6.3. Methods and material for containment and cleaning up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

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

7.2. Conditions for safe storage, including any incompatibilities

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Keep containers tightly closed in a dry, cool and well-ventilated place.

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies.

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.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Derived No Effect Level (DNEL) No information available

Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral Dermal Inhalation				

Predicted No Effect Concentration (PNEC) No information available.

8.2. Exposure controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

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 Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

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Skin and body protection Long sleeved clothing

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 compatability, 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.

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

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: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Appearance

Physical State Liquid

Odor

Odorless

Odor Threshold

No data available

pH

No information available

Melting Point/Range

No data available

Softening Point

No data available

Boiling Point/Range

135 - 140 °C / 275 - 284 °F

@ 10 mmHg

Flash Point

No information available

Method - No information available

Evaporation Rate

No data available

Flammability (solid,gas)

Not applicable

Liquid

Explosion Limits

No data available

Vapor Pressure

No data available

Vapor Density

No data available

(Air = 1.0)

Specific Gravity / Density

1.03

Bulk Density

Not applicable

Liquid

Water Solubility

Insoluble

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

No data available

Explosive Properties

No information available

Oxidizing Properties

No information available

9.2. Other information

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Molecular Formula C12 H13 N
Molecular Weight 171.24

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity
None known, based on information available

10.2. Chemical stability
Stable under normal conditions

10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid
Incompatible products. Excess heat.

10.5. Incompatible materials
Strong oxidizing agents.

10.6. Hazardous decomposition products
Nitrogen oxides (NO_x). Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on toxicological effects

Product Information

- (a) acute toxicity;
- | | |
|------------|------------|
| Oral | Category 4 |
| Dermal | Category 4 |
| Inhalation | Category 4 |
- (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
- (i) STOT-repeated exposure; No data available
- | | |
|---------------|---------------------------|
| Target Organs | No information available. |
|---------------|---------------------------|
- (j) aspiration hazard; No data available

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Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed No information available

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects Do not empty into drains.

12.2. Persistence and degradability

Persistence Insoluble in water, Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential

May have some potential to bioaccumulate

12.4. Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and sinks in water The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility.

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Other adverse effects

Endocrine Disruptor Information
Persistent Organic Pollutant
Ozone Depletion Potential

This product does not contain any known or suspected endocrine disruptors
This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

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.

European Waste Catalogue (EWC)

According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.

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

IMDG/IMO

14.1. UN number

UN3276

14.2. UN proper shipping name

Nitriles, toxic, n.o.s

14.3. Transport hazard class(es)

6.1

14.4. Packing group

III

ADR

14.1. UN number

UN3276

14.2. UN proper shipping name

Nitriles, toxic, n.o.s

14.3. Transport hazard class(es)

6.1

14.4. Packing group

III

IATA

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14.1. UN number	UN3276
14.2. UN proper shipping name	Nitriles, toxic, n.o.s
14.3. Transport hazard class(es)	6.1
14.4. Packing group	III
14.5. Environmental hazards	No hazards identified
14.6. Special precautions for user	No special precautions required
14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories		X = listed									
Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	IECSC	AICS	KECL
1-Phenylcyclohexanecarbonitril e	201-038-2	-		-	-	-	-	X	-	-	-

National Regulations

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment.
Take note of Dir 94/33/EC on the protection of young people at work
Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full Text of H-/EUH-Statements Referred to Under Section 3

H302 - Harmful if swallowed
H312 - Harmful in contact with skin
H332 - Harmful if inhaled
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

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ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - Volatile Organic Compounds

Key literature references and sources for data

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

Training Advice

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

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

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Revision Summary Update to Format.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

Disclaimer

The information provided on 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 guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as 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 material or in any process, unless specified in the text.

End of Safety Data Sheet