

Chemical Safety Data Sheet MSDS / SDS

PACOCF3

Revision Date:2026-07-18 Revision Number:1

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

Product identifier

Product name : PACOCF3
CBnumber : CB8430016
CAS : 141022-99-3
Synonyms : ptk,Palmityl Trifluoromethyl Ketone

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

Danger

Precautionary statements

P202 Do not handle until all safety precautions have been read and understood.
P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352 IF ON SKIN: wash with plenty of soap and water.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308+P313 IF exposed or concerned: Get medical advice/attention.

Hazard statements

H315 Causes skin irritation
H319 Causes serious eye irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: PACOCF3
Synonyms	: ptk, Palmityl Trifluoromethyl Ketone
CAS	: 141022-99-3
MF	: C17H31F3O
MW	: 308.42

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NOx)

Oxides of phosphorus

Hydrogen chloride gas

Sodium oxides

Hydrogen cyanide (hydrocyanic acid)

Mixture with combustible ingredients.

Development of hazardous combustion gases or vapours possible in the event of fire.

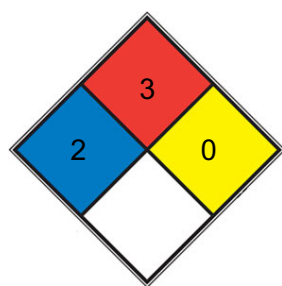
5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

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

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-

absorbent material (e.g.

Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stabilityRecommended storage temperature

-70 °C

Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-

approved gloves (e.g. KCL GmbH, D-36124 Eichenzell,

Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested:KCL 741 L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested:KCL 741 L

Body Protection

protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	Aqueous solution
b) Color	White to off-white
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	329.0±37.0 °C(Predicted)
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	14 °C
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available

m) Water solubility	at 20 °C soluble
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	0.955±0.06 g/cm ³ (Predicted)
Relative density	0.955±0.06 g/cm ³ (Predicted)
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none
Solubility	Soluble in DMSO

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

The generally known reaction partners of water.

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong bases, Bases, Oxidizing agents, Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture Acute toxicity

Oral: No data available

Symptoms: Possible symptoms:, mucosal irritations

Dermal: No data available

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

May harm the unborn child.

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information**Endocrine disrupting properties**

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

prolonged or repeated exposure can cause:, Nausea, Dizziness

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components Imidazole**Acute toxicity**

LD50 Oral - Rat - 970 mg/kg (OECD Test Guideline 401)

Acute toxicity estimate Oral - 970 mg/kg (ATE value derived from LD50/LC50 value)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive after 1 to 4 hours of exposure - 4 h (OECD Test Guideline 404)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage.

(OECD Test Guideline 405)

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Test Type: unscheduled DNA synthesis assay

Test system: rat hepatocytes

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Bone marrow

Result: negative

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

May damage the unborn child.

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Oral - Liver, Kidney

Aspiration hazard

Classified based on available data. For more details, see section 2

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission

Delegated regulation (EU) 2017/2100 or Commission

Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

No data available

Components Imidazole

Toxicity to daphnia static test EC50 - Daphnia magna (Water flea) - 341,5 mg/l - and other aquatic 48 h invertebrates (Regulation (EC) No. 440/2008, Annex, C.2)

Toxicity to algae static test ErC50 - Desmodesmus subspicatus (green algae) - 133 mg/l - 72 h (DIN 38412)

Toxicity to bacteria static test EC50 - activated sludge - > 1.000 mg/l - 30 min (OECD Test Guideline 209)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: -

IMDG: -

IATA: -

14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA: -

14.4 Packaging group

ADR/RID: -

IMDG: -

IATA: -

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

No data available

Further information: Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

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

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

Authorisations and/or restrictions on use

REACH - Restrictions on the manufacture, : Imidazole placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII)

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR - Agreement concerning the International Carriage of Dangerous Goods by Road

AIRC - Australian Inventory of Industrial Chemicals

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)
 ErCx -Concentration associated with x% growth rate response
 GHS - Globally HarmonizedSystem
 GLP - Good Laboratory Practice
 IARC - International Agency for Research onCancer
 IATA - International Air Transport Association
 IBC - International Code for theConstruction and Equipment of Ships carrying Dangerous Chemicals in Bulk
 IC50 - Half maximal inhibitory concentration
 ICAO - International Civil Aviation Organization
 IECSC - Inventory of Existing Chemical Substances in China
 IMDG - InternationalMaritime Dangerous Goods
 IMO - International Maritime Organization
 ISHL - IndustrialSafety and Health Law (Japan)
 ISO - International Organisation for Standardization
 KECI - Korea Existing Chemicals Inventory
 LC50 - Lethal Concentration to 50 % of a test population
 LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)
 MARPOL - International Convention for the Prevention of Pollution from Ships
 n.o.s. -Not Otherwise Specified
 NO(A)EC - No Observed (Adverse) Effect Concentration
 NO(A)EL - No Observed (Adverse) Effect Level
 NOELR - No Observable Effect LoadingRate
 NZIoC - New Zealand Inventory of Chemicals
 OECD - Organization for EconomicCo-operation and Development
 OPPTS - Office of Chemical Safety and PollutionPrevention
 PBT - Persistent, Bioaccumulative and Toxic substance
 PICCS - PhilippinesInventory of Chemicals and Chemical Substances
 (Q)SAR - (Quantitative) StructureActivity Relationship
 REACH - Regulation (EC) No 1907/2006 of the EuropeanParliament and of the Council concerning the Registration, Evaluation, Authorisation andRestriction of Chemicals
 RID - Regulations concerning the International Carriage ofDangerous Goods by Rail
 SADT - Self-Accelerating Decomposition Temperature
 SDS -Safety Data Sheet
 TCSI - Taiwan Chemical Substance Inventory
 TECI - ThailandExisting Chemicals Inventory
 TSCA - Toxic Substances Control Act (United States)
 UN - United Nations
 UNRTDG - United Nations Recommendations on the Transport ofDangerous Goods
 vPvB - Very Persistent and Very Bioaccumulative

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.

