Chemical Safety Data Sheet MSDS / SDS

Diacetone Alcohol

Revision Date:2025-03-01 Revision Number:1

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

Product identifier

Product name : Diacetone Alcohol

CBnumber : CB9783177

CAS : 123-42-2

EINECS Number : 204-626-7

Synonyms : Diacetone alcohol, DAA

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

P403+P235 Store in a well-ventilated place. Keep cool.

P370+P378 In case of fire: Use ... for extinction.

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

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P240 Ground/bond container and receiving equipment.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H319 Causes serious eye irritation

H303 May be harmfulif swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name : Diacetone Alcohol
Synonyms : Diacetone alcohol,DAA

CAS : 123-42-2
EC number : 204-626-7
MF : C6H12O2
MW : 116.16

SECTION 4: First aid measures

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.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media

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

Special hazards arising from the substance or mixture

Carbon oxides Combustible.

Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air at elevated temperatures.

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

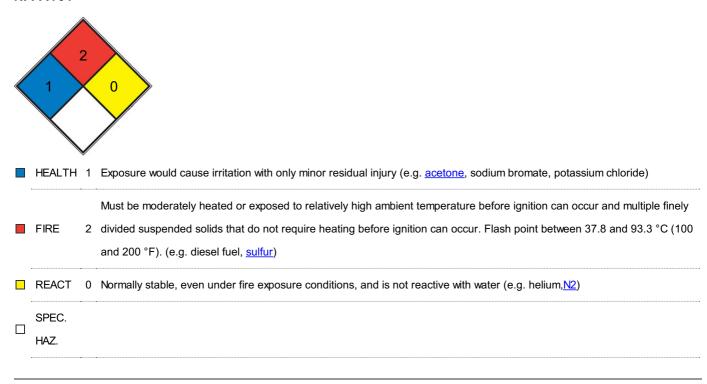
Advice for firefighters

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

Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

NFPA 704



SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

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 with liquid-absorbent material (e.g. Chemizorb?). Dispose of properly. Clean up affected area.

Reference to other sections

SECTION 7: Handling and storage

Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,7 mm Break through time: 480 min Material tested:Butoject? (KCL 898)

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact Material: Chloroprene

Minimum layer thickness: 0,65 mm Break through time: 240 min Material tested: KCL 720 Camapren?

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepeneur 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. Risk of explosion.

Exposure limits

TLV-TWA 240 mg/m³ (50 ppm) (ACGIH); IDLH 2100 ppm (NIOSH).

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	light yellow clear, liquid
Odour	No data available
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	Melting point: -44 °C
Initial boiling point and boiling range	166 °C - lit.
Flash point	58 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	Upper explosion limit: 6,9 %(V) Lower explosion limit: 1,8 %(V)
limits	
Vapour pressure	<1 mm Hg (20 °C)
Vapour density	4,01 - (Air = 1.0)
Relative density	No data available
Water solubility	Soluble in alcohol, ether (Weast, 1986), and many other solvents, particular ketones such as
	acetone and 2-butanone.
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available
λmax	249nm(lit.)
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Other safety information

Relative vapor density

SECTION 10: Stability and reactivity

Reactivity

Vapor/air-mixtures are explosive at intense warming.

Chemical stability

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

Possibility of hazardous reactions

No data available

Conditions to avoid

Heating.

Incompatible materials

various plastics, Strong oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 3.002 mg/kg

(OECD Test Guideline 401)

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

Symptoms: mucosal irritations

LD50 Dermal - Rabbit - 13.630 mg/kg Remarks: (IUCLID)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h (OECD Test Guideline 404) Remarks: (IUCLID)

Drying-out effect resulting in rough and chapped skin. Dermatitis

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes. (OECD Test Guideline 405) Remarks: (IUCLID)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation Method: OECD Test Guideline

471

Result: negative

Test Type: In vitro mammalian cell gene mutation test Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 476

Result: negative

Test Type: Chromosome aberration test in vitro Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 473

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging the unborn child. Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause respiratory irritation. - Respiratory Tract

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Toxicity

LD50 orally in rats: 4.0 g/kg (Smyth)

SECTION 12: Ecological information

Toxicity

Toxicity to fish

semi-static test LC50 - Oryzias latipes (Orange-red killifish) - > 100 mg/l - 96 h

(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 - Daphnia magna (Water flea) - > 1.000 mg/l

- 48 h

(OECD Test Guideline 202)

semi-static test NOEC - Daphnia magna (Water flea) - > 1.000 mg/l

- 48 h

(OECD Test Guideline 202)

Toxicity to algae

static test ErC50 - Pseudokirchneriella subcapitata (green algae) - >

1.000 mg/l - 72 h

(OECD Test Guideline 201)

static test NOEC - Pseudokirchneriella subcapitata (green algae) - >=

1.000 mg/l - 72 h

(OECD Test Guideline 201)

Toxicity to bacteria

static test EC50 - activated sludge - > 1.000 mg/l - 3 h (OECD Test Guideline 209)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 98,51 % - Readily biodegradable. (OECD Test Guideline 301A)

Bioaccumulative potential

No data available

Mobility in soil

No data available

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.

Toxics Screening Level

The final Initial Threshold Screening Level (ITSL) for diacetone alchohol is 2375 µg/m3 based on an 8-hour averaging time.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

Incompatibilities

Vapor may form explosive mixture with air. Incompatible with oxidizers (chlorates, nitrates, perox- ides, permanganates, perchlorates, chlorine, bromine, fluo- rine, etc.); contact may cause fires or explosions. Keep away from alkaline materials, strong bases, strong acids, oxoacids, and epoxides.

Waste Disposal

Dissolve or mix the material with a combustible solvent and burn in a chemical incinera- tor equipped with an afterburner and scrubber. All federal, state, and local environmental regulations must be observed.

SECTION 14: Transport information

UN number

ADR/RID: IMDG: 1148 IATA: 1148

UN proper shipping name

ADR/RID:

IMDG: DIACETONE ALCOHOL

IATA: Diacetone alcohol

Transport hazard class(es)

ADR/RID: IMDG: 3 IATA: 3

Packaging group

ADR/RID: IMDG: III IATA: III

Environmental hazards

ADR/RID: IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/

Korea Existing Chemicals List (KECL):Listed. website: http://ncis.nier.go.kr

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: https://www.mee.gov.cn/

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

New Zealand Inventory of Chemicals (NZIoC):Listed. website: https://www.epa.govt.nz/

EC Inventory:Listed.

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

- [1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- [2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- [3] ECHA European Chemicals Agency, website: https://echa.europa.eu/
- [4] eChemPortal The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

- [5] ERG Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- [6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- [7] HSDB Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- [8] IARC International Agency for Research on Cancer, website: http://www.iarc.fr/
- [9] IPCS The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- [10] Sigma-Aldrich, website: https://www.sigmaaldrich.com/

Other Information

This card is only valid for the pure substance. The technical product may contain up to 5% acetone (see ICSC 0087), resulting in high flammability. Other UN Classification for technical product: UN hazard class 3, UN pack group II.

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.