GPS Safety Summary

Contacts

Diacetone alcohol

Chemical Identity

Brand names	**Diacetone alcohol**	*CAS number*	**123-42-2**
Chemical name (IUPAC)	**4-Hydroxy-4-methylpentan-2-one**	*Molecular formula*	**$C_6H_{12}O_2$**
Synonyms	**DAA; 2-Methyl-2-pentanol-4-one; Diacetonic alcohol**	*Molecular weight*	**116.16 g/mol**

Applications

Diacetone alcohol is mainly used as a solvent in industrial and professional applications in coatings, cleaning, oil and gas filed drilling, lubricants, metal working fluids, polymer processing and water treatment. It is found in a number of consumer products such as adhesives, inks, paints, household cleaners and agrochemicals. The substance is also a chemical intermediate for the preparation of other compounds.

Safety Assessment, Exposure and Risk Management Recommendations

Physical and chemical properties

Property	Result
Physical state	Liquid
Colour	Colourless
Odour	Slight
Boiling point	168°C
Relative density	0.94 at 20°C
Flash point	42 to 63°C (closed cup)*
Vapour pressure	Low potential for volatility
Water solubility	Soluble
Octanol water partition	Low potential for bioaccumulation

Health effects

Diacetone alcohol causes serious eye irritation and may be irritating to the upper respiratory tract. For industrial uses, stringent safety measures must be observed. For more details, please refer to the Safety Data Sheet.
For consumer applications, it is used in suitable concentrations according to appropriate regulations.

Environmental effects

Diacetone alcohol is readily biodegradable and not potentially bioaccumulable. It is not classified as dangerous for the environment.
Disposal, treatment or recycling must comply with applicable regulations to preserve the environment.

Regulatory and certification information

*Classification and labelling**

EU regulation (EC) 1272/2008 (CLP)

Flammable liquids, Cat.3 — H226 Flammable liquid and vapour.

Eye irritation, Cat.2 — H319 Causes serious eye irritation.
STOT single exposure, Cat.3 — H335 May cause respiratory irritation.

Warning

*Depending on its purity, the flash point of DAA varies from 42 to 63°C. Accordingly, the substance may or may not be classified as “flammable” according to EU regulation 1272/2008 (CLP).

Registration and certification

ISO 9001: 2008
EU regulation for chemicals (EC) 1907/2006 (REACH)

Diacetone alcohol is formulated to comply with requirements of most stringent regulations for applicable consumer uses. It can be safely used in suitable concentrations according to appropriate regulations.

GPS Safety Summary

This Product Safety Summary is intended to provide a general overview of the chemical substance in the context of ICCA Global Product Strategy. The information on the Summary is basic information and is not intended to provide emergency response information, medical information or treatment information. The summary should not be used to provide in-depth safety and health information. In-depth safety and health information can be found on the (extended) Safety Data Sheet (e)SDS for the chemical substance.

Diacetone alcohol

General Statement

Diacetone alcohol is a colourless liquid organic compound with a slight odour, soluble in water, oil and in common organic solvents.

Diacetone alcohol is a well-known synthetic intermediate and it occurs as a component in a large number of products for industrial, professional and consumer uses such as coatings, paints, cleaning products or agrochemicals.

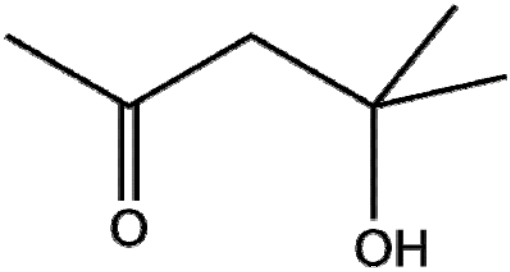
The pure substance is a flammable liquid. It causes serious eye irritation and may be irritating to the upper respiratory tract. It is professionally or industrially used and must be handled under stringent safety conditions in accordance with the risk management measures to keep the exposure at a safe level and to preserve human health and environment.

Diacetone alcohol is formulated in suitable concentrations for consumer applications, according to appropriate regulations, to ensure safe use of the final product, in the conditions of use written on the product packaging.

Chemical Identity

Name:	Diacetone alcohol
Brand names:	Diacetone alcohol
Chemical name (IUPAC):	4-Hydroxy-4-methylpentan-2-one
Synonyms:	DAA; 2-Methyl-2-pentanol-4-one; Diacetonic alcohol; Dimethylacetonilcarbinol; Pyranton A; 4-Hydroxy-2-ceto-4-methyl-pentane
CAS number(s):	123-42-2
EC number:	204-626-7
Molecular formula:	$C_6H_{12}O_2$

Structure:



Uses and applications

Diacetone alcohol is a low evaporating solvent with high water solubility. It is widely used in industrial and professional applications in coatings, cleaning, oil and gas field drilling, lubricants, metal working fluids, polymer processing and water treatment. It is also used as chemical intermediate in organic synthesis.

Diacetone alcohol is also used as solvent in consumer products such as adhesives, inks, paints, thinners, paint removers, household cleaners and agrochemicals.

Physical/Chemical Properties

Phys/Chem Safety Assessment

Property	Value
Physical state	Liquid at 20°C and atmospheric pressure
Colour	Colourless
Odour	Slight odour
Molecular weight	116.16 g/mol
Relative density	0.940 at 20°C
Melting Point	- 44°C
Boiling Point	168°C at atmospheric pressure
Flash point	42 to 63°C (closed cup)
Explosive properties	Non explosive properties expected
Self-ignition temperature	643°C
Vapour pressure	1.29 hPa at 20°C
Water solubility	Soluble in water
Octanol Water partition coefficient (log Kow)	- 0.09 at room temperature Low potential for bioaccumulation

Depending on its purity, the flash point of diacetone alcohol varies from 42 to 63°C. Accordingly, the substance may or may not be classified as "flammable" according to EU regulation (EC) 1272/2008 (upper cut-off value of 60°C for classification of liquid substances as "flammable" under this regulation).

Health Effects

Human Health Safety Assessment

Effect Assessment	Result
Acute Toxicity Oral/inhalation/dermal	Low toxicity in rats following oral exposure, dermal exposure and inhalation, not resulting in classification
Irritation / corrosion Skin/eye/respiratory tract	Irritating for the eyes and for the respiratory tract Not irritating for the skin
Sensitisation	No skin sensitizing properties
Toxicity after repeated exposure Oral/inhalation/dermal	No significant toxicity following long-term oral or inhalation administration to laboratory rats No data available by dermal route of exposure
Genotoxicity / Mutagenicity	No genetic toxicity based on several *in vitro* study results
Carcinogenicity	No carcinogenic effects relevant to humans expected, by analogy with methyl isobutyl ketone
Toxicity for reproduction	No adverse effect on fertility and on development based on *in vivo* experimental study results and by analogy with methyl isobutyl ketone

Diacetone alcohol is subject to harmonised classification and labelling in accordance with annex VI table 3.1., EU regulation (EC) 1272/2008. According to annex VI it is classified as irritating to the eyes, however, a study showed that it is also irritating for the respiratory tract. Therefore, diacetone alcohol should be reclassified as substance which causes serious eye irritation and which may cause respiratory irritation, according to EU regulation (EC) 1272/2008 criteria.

Environmental Effects

Environment Safety Assessment

Effect Assessment	Result
Aquatic Toxicity	Not hazardous to fish, invertebrates and algae

Fate and behaviour	Result
Biodegradation	Readily biodegradable
Bioaccumulation potential	Not potentially bioaccumulative (Log Kow = - 0.09)
PBT / vPvB conclusion	Not considered to be either PBT or vPvB

Based on available data, diacetone alcohol is not considered as dangerous for aquatic organisms. Readily biodegradable and not potentially bioaccumulative, it is not classified as dangerous for the environment according to EU regulation (EC) 1272/2008.

Exposure

Considering the diacetone alcohol lifecycle, from its manufacture to its end-use, the implementation of risk management measures ensure that the potential for human and environment exposure is at a safe level.

Human health

The most relevant routes of exposure for workers are skin contact and inhalation. On manufacturing, industrial or professional sites, diacetone alcohol is handled as much as possible in closed systems which ensure that the risk is controlled. Where there is a risk of exposure, during (un)loading, mixing, sampling, analysis or maintenance operations, and particularly in case of batch processes and spray applications, it must be kept as low as possible and at a safe level (strictly below exposure limits, when applied) by the use of appropriate risk management measures as suitable collective and personal protective equipment, good industrial hygiene practices and risk communication through appropriate training of workers.

In end-use products like paints, cleaners or agrochemicals, diacetone alcohol is formulated to comply with requirements of the most stringent regulations for all applicable consumer uses to ensure that final products are used safely in the conditions of use written on the packaging.

Environment

Based on its physico-chemical properties, diacetone alcohol is water soluble, has a low potential for bioaccumulation and is readily biodegradable. It would be expected to partition predominantly into the aquatic compartment and not to adsorb on soil or sediment particles. In addition it is not persistent.
Emissions in the air are not expected as diacetone alcohol has a low potential for volatility.

On industrial manufacturing and professional sites, effluents that may contain the substance must be directed to a waste water treatment plant.

Due to its ecological properties, an indirect exposure of humans to diacetone alcohol via the environment is not expected.

Risk Management Recommendations

For industrial, professional and consumer uses of diacetone alcohol, recommendations to preserve human health and environment are based on the risk assessment, for each exposure scenario along the substance life-cycle.

Human health

For industrial and professional uses of diacetone alcohol and as recommended for the use of any chemical product, workers must be well informed and trained and must refer to the extended Safety Data Sheet (eSDS).
Where there is a risk of exposure to the substance (during (un)loading, mixing, sampling, analysis or maintenance operations and particularly in case of batch processes and spray applications), it must be controlled by handling the substance under an adequate and efficient ventilation, appropriate Personal Protective Equipment (PPE) must be worn (tightly fitting safety goggles, chemically resistant gloves, protective suit) as recommended in the eSDS. In case of exposure to vapour or aerosol, a respirator with

approved filter should be used. General industrial hygiene measures are required to ensure safe handling of the substance: Use well-maintained PPE; wash hands and skin following contact; do not eat, drink or smoke at the workplace.

Diacetone alcohol being a flammable liquid, appropriate measures must be implemented to control the risk: Use only in well-ventilated areas, keep away from ignition sources, use explosion-proof equipment.

For consumer uses, diacetone alcohol is formulated in suitable concentrations according to appropriate regulations, to ensure safe-use of the final products, in the conditions of use written on the product packaging.
For specific products meant to be used by consumers, please contact your supplier.

Environment

All industrial aqueous releases that may contain the substance must be directed to a waste water treatment plant.
Disposal, treatment or recycling of industrial waste must comply with applicable regulations to preserve environment.

State Agency Review

Diacetone alcohol has been registered under:	EU regulation (EC) 1907/2006 (REACH)
Diacetone alcohol has been reviewed under the following regulatory and/or voluntary programmes:	High Production Volume chemicals programme, published by UNEP in 2002

Diacetone alcohol substance meets the requirements of the most stringent regulations for all applicable consumer applications.

Regulatory Information / Classification and Labelling

Substance classification and labelling according to EU regulation (EC) 1272/2008 (CLP):

Adjusted classification*

Flammable liquids, Category 3	H226 Flammable liquid and vapour.
Eye irritation, Category 2	H319 Causes serious eye irritation.
Specific target organ toxicity - single exposure, Category 3	H335 May cause respiratory irritation.

Adjusted Labelling*

Pictogram:

Signal word: Warning

Hazard statements:

H319 Causes serious eye irritation.
H226 Flammable liquid and vapour.
H335 May cause respiratory irritation.

Precautionary statements:

P233 Keep container tightly closed.
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 IF INHALED: Remove victim 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.
P311 Call a POISON CENTER or doctor/ physician.
P403 + P235 Store in a well-ventilated place. Keep cool.

*Harmonised EU classification and labelling, adjusted by Rhodia based on available data.
Depending on its purity, the flash point of diacetone alcohol varies from 42 to 63°C. As the upper cut-off value for classification of liquid substances as "flammable" under EU regulation 1272/2008 is 60°C, diacetone alcohol in high purity is not classified for flammability (flash point >= 61°C).

Contact information within company

For further information on this substance or Product Safety Summaries in general, please contact:

Rhodia Global Product Strategy: http://www.rhodia.com/en/sustainability/global_product_strategy/index.tcm

Contact: globalproductstrategy@eu.rhodia.com

Additional information

ICCA Global Product Strategy: http://www.icca-chem.org/en/Home/ICCA-initiatives/global-product-strategy/

(extended) Safety Data Sheet available on demand: http://www.rhodia.com/en/contact/contact_form_business.tcm

Glossary of technical terms: http://www.rhodia.com/en/sustainability/global_product_strategy/glossary/index.tcm

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Disclaimer

The information provided in the present Safety Summary is based on European data available in REACH regulatory dossier (EC N°1907/2006) and is correct to the best of our knowledge, information and belief at the date of its publication. Such information is only intended to provide a general overview of the chemical substance in the context of ICCA Global Product Strategy and is not to be considered as a warranty or quality specification. It does not replace the safety data sheet and technical sheets. Thus, the information provided in this Safety Summary only relates to the designated specific product and may not be applicable if such product is used in combination with other materials or in another manufacturing process, unless otherwise specifically indicated. It does not release the user from ensuring he is in conformity with all regulations linked to its activity.