

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

1.1. Product identifier

Product form	: Substance
Substance name	: acetone-D6
EC index no	: 606-001-00-8
EC no	: 211-563-9
CAS No.	: 666-52-4
Product code	: D009, D030, D038, DLM-9
Formula	: C3D6O
Synonyms	: (-(2)-H6)acetone / 2-propanone, 1,1,1,3,3,3-D6 / hexadeuteroacetone

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

1.2.1. Relevant identified uses

Main use category	: Professional use
Use of the substance/preparation	: NMR solvent
Function or use category	: Laboratory chemicals for research

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

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91194 Saint-Aubin CEDEX - France - FRANCE
T +33 1 69 41 97 98 - F +33 1 69 41 93 52
eurisotop@eurisotop.com - www.eurisotop.com

1.4. Emergency telephone number

Country	Official advisory body	Address	Emergency number
UNITED KINGDOM	Guy's & St Thomas' Poisons Unit Medical Toxicology Unit, Guy's & St Thomas' Hospital Trust	Avonley Road SE14 5ER London	0870 243 2241

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Flam. Liq. 2 H225
Eye Irrit. 2 H319
STOT SE 3 H336

Full text of H-phrases: see section 16.

Classification according to Directive 67/548/EEC or 1999/45/EC

F; R11
Xi; R36
R67
R66

Full text of R-phrases: see section 16.

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP)



GHS02

GHS07

CLP Signal word	: Danger
Hazard statements (CLP)	: H225 - Highly flammable liquid and vapour H319 - Causes serious eye irritation H336 - May cause drowsiness or dizziness
EUH phrases	: EUH066 - Repeated exposure may cause skin dryness or cracking

2.3. Other hazards

No additional information available

acetone-D6

Safety Data Sheet

according to Regulation (EC) No. 453/2010

SECTION 3: Composition/information on ingredients

3.1. Substances

Name	Product identifier	%	Classification according to Directive 67/548/EEC
acetone-D6 (Main constituent)	(CAS No.) 666-52-4 (EC no) 211-563-9 (EC index no) 606-001-00-8	100	F; R11 Xi; R36 R67 R66

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
acetone-D6 (Main constituent)	(CAS No.) 666-52-4 (EC no) 211-563-9 (EC index no) 606-001-00-8	100	Flam. Liq. 2, H225 Eye Irrit. 2, H319 STOT SE 3, H336

Full text of R-, H- and EUH-phrases: see section 16.

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: Check the vital functions. Unconscious: maintain adequate airway and respiration. Respiratory arrest: artificial respiration or oxygen. Cardiac arrest: perform resuscitation. Victim conscious with laboured breathing: half-seated. Victim in shock: on his back with legs slightly raised. Vomiting: prevent asphyxia/aspiration pneumonia. Prevent cooling by covering the victim (no warming up). Keep watching the victim. Give psychological aid. Keep the victim calm, avoid physical strain. Depending on the victim's condition: doctor/hospital.
First-aid measures after inhalation	: Remove the victim into fresh air. Respiratory problems: consult a doctor/medical service.
First-aid measures after skin contact	: Wash immediately with lots of water. Do not apply (chemical) neutralizing agents. Take victim to a doctor if irritation persists.
First-aid measures after eye contact	: Rinse immediately with plenty of water. Do not apply neutralizing agents. Take victim to an ophthalmologist if irritation persists.
First-aid measures after ingestion	: Rinse mouth with water. Do not induce vomiting. Call Poison Information Centre (www.big.be/antigif.htm). Consult a doctor/medical service if you feel unwell. Ingestion of large quantities: immediately to hospital.

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

Symptoms/injuries after inhalation	: EXPOSURE TO HIGH CONCENTRATIONS: Feeling of weakness. CNS depression. Dizziness. Narcosis. Excited/restless. Drunkenness. Disturbed motor response. Headache. Respiratory difficulties. Disturbances of consciousness. Irritation of the respiratory tract. Vomiting. Nausea.
Symptoms/injuries after skin contact	: ON CONTINUOUS EXPOSURE/CONTACT: Dry skin. Cracking of the skin.
Symptoms/injuries after eye contact	: Irritation of the eye tissue.
Symptoms/injuries after ingestion	: Dry/sore throat. Risk of aspiration pneumonia. Symptoms similar to those listed under inhalation. AFTER ABSORPTION OF HIGH QUANTITIES: Irritation of the gastric/intestinal mucosa. Change in the haemogramme/blood composition. Change in urine output.
Chronic symptoms	: ON CONTINUOUS/REPEATED EXPOSURE/CONTACT: Red skin. Skin rash/inflammation. Dry/sore throat. Headache. Nausea. Feeling of weakness. Loss of weight. Risk of aspiration pneumonia.

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

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	: Alcohol-resistant foam. Polymer foam. BC powder. Carbon dioxide.
Unsuitable extinguishing media	: Solid water jet ineffective as extinguishing medium.

5.2. Special hazards arising from the substance or mixture

Fire hazard	: DIRECT FIRE HAZARD. Highly flammable. Gas/vapour flammable with air within explosion limits. INDIRECT FIRE HAZARD. May be ignited by sparks. Gas/vapour spreads at floor level: ignition hazard.
Explosion hazard	: DIRECT EXPLOSION HAZARD. Gas/vapour explosive with air within explosion limits. INDIRECT EXPLOSION HAZARD. Heat may cause pressure rise in tanks/drums: explosion risk. may be ignited by sparks.
Reactivity	: Upon combustion CO and CO2 are formed.

5.3. Advice for firefighters

Firefighting instructions	: Cool tanks/drums with water spray/remove them into safety. Physical explosion risk: extinguish/cool from behind cover. Do not move the load if exposed to heat. After cooling: persistent risk of physical explosion.
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acetone-D6

Safety Data Sheet

according to Regulation (EC) No. 453/2010

Protection during firefighting : Heat/fire exposure: compressed air/oxygen apparatus.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Protective equipment : Gloves. Protective goggles. Protective clothing. Large spills/in enclosed spaces: compressed air apparatus. See "Material-Handling" to select protective clothing.

Emergency procedures : Keep upwind. Mark the danger area. Consider evacuation. Seal off low-lying areas. Close doors and windows of adjacent premises. Stop engines and no smoking. No naked flames or sparks. Spark- and explosionproof appliances and lighting equipment. Keep containers closed. Wash contaminated clothes.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent spreading in sewers.

6.3. Methods and material for containment and cleaning up

For containment : Contain released substance, pump into suitable containers. Plug the leak, cut off the supply. Dam up the liquid spill. Try to reduce evaporation. Measure the concentration of the explosive gas-air mixture. Dilute/disperse combustible gas/vapour with water curtain. Provide equipment/receptacles with earthing. Do not use compressed air for pumping over spills.

Methods for cleaning up : Take up liquid spill into absorbent material, e.g.: activated carbon or sand/earth. Scoop absorbed substance into closing containers. Carefully collect the spill/leftovers. Damaged/cooled tanks must be emptied. Do not use compressed air for pumping over spills. Clean contaminated surfaces with an excess of water. Take collected spill to manufacturer/competent authority. Wash clothing and equipment after handling.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Comply with the legal requirements. Remove contaminated clothing immediately. Clean contaminated clothing. Handle uncleaned empty containers as full ones. Do not discharge the waste into the drain. Do not use compressed air for pumping over. Use spark-/explosionproof appliances and lighting system. Take precautions against electrostatic charges. Keep away from naked flames/heat. Keep away from ignition sources/sparks. Avoid prolonged and repeated contact with skin. Keep container tightly closed. Measure the concentration in the air regularly. Work under local exhaust/ventilation.

7.2. Conditions for safe storage, including any incompatibilities

Heat-ignition : KEEP SUBSTANCE AWAY FROM: heat sources. ignition sources.

Prohibitions on mixed storage : KEEP SUBSTANCE AWAY FROM: oxidizing agents. reducing agents. (strong) bases. metals.

Storage area : Store in a cool area. Keep out of direct sunlight. Store in a dry area. Ventilation at floor level. Provide for a tub to collect spills. Provide the tank with earthing. May be stored under nitrogen. Meet the legal requirements.

Special rules on packaging : SPECIAL REQUIREMENTS: closing, opaque, correctly labelled, meet the legal requirements. Secure fragile packagings in solid containers.

Packaging materials : SUITABLE MATERIAL: Glass. MATERIAL TO AVOID: No data available.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

acetone-D6 (666-52-4)		
EU	IOELV TWA (mg/m ³)	1210 mg/m ³
EU	IOELV TWA (ppm)	500 ppm
France	VLE (mg/m ³)	2420 mg/m ³
France	VLE (ppm)	1000 ppm
France	VME (mg/m ³)	1210 mg/m ³
France	VME (ppm)	500 ppm
United Kingdom	WEL TWA (mg/m ³)	1210 mg/m ³
United Kingdom	WEL TWA (ppm)	500 ppm
United Kingdom	WEL STEL (mg/m ³)	3620 mg/m ³
United Kingdom	WEL STEL (ppm)	1500 ppm

acetone-D6

Safety Data Sheet

according to Regulation (EC) No. 453/2010

8.2. Exposure controls

Materials for protective clothing	: GIVE EXCELLENT RESISTANCE: butyl rubber. GIVE GOOD RESISTANCE: chlorosulfonated polyethylene. neoprene. GIVE POOR RESISTANCE: viton.
Hand protection	: Gloves.
Eye protection	: Protective goggles.
Skin and body protection	: Head/neck protection. Protective clothing.
Respiratory protection	: Wear gas mask with filter type A if conc. in air > exposure limit.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Liquid.
Molecular mass	: 64.12 g/mol
Colour	: No data available on colour.
Odour	: Characteristic odour.
Odour threshold	: No data available
pH	: No data available
Melting point	: -94 °C
Solidification point	: No data available
Boiling point	: 55 °C
Flash point	: -17 °C
Relative evaporation rate (butylacetate=1)	: No data available
Flammability (solid, gas)	: No data available
Explosive limits	: 2.16 - 13.2 vol %
Vapour pressure	: 245 hPa (20 °C)
Vapour pressure at 50 °C	: <= 1100 hPa (50 °C)
Relative vapour density at 20 °C	: 2
Relative density	: 0.87
Density	: 872 kg/m ³
Solubility	: Literature reports: soluble in water.
Log Pow	: -0.24 (exp.)
Log Kow	: No data available
Self ignition temperature	: 464 °C
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: 0.00034 Pa.s (22 °C)
Explosive properties	: No data available
Oxidising properties	: No data available

9.2. Other information

VOC content	: 100 %
Other properties	: Gas/vapour heavier than air at 20°C. Highly volatile.

SECTION 10: Stability and reactivity

10.1. Reactivity

Upon combustion CO and CO₂ are formed.

10.2. Chemical stability

Unstable on exposure to light.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

No additional information available

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

No additional information available

acetone-D6

Safety Data Sheet

according to Regulation (EC) No. 453/2010

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

acetone-D6 (666-52-4)	
LD50 oral rat	9750 mg/kg

Skin corrosion/irritation : Not classified
Serious eye damage/irritation : Causes serious eye irritation.
Respiratory or skin sensitisation : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
Specific target organ toxicity (single exposure) : May cause drowsiness or dizziness.
Specific target organ toxicity (repeated exposure) : Not classified
Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Classification concerning the environment: not applicable.
Ecology - air : Not dangerous for the ozone layer (Council Regulation (EC) no 1005/2009). Germany: TA-Luft Klasse 5.2.5.
Ecology - water : Mild water pollutant (surface water). Not harmful to fishes (LC50(96h) >1000 mg/l). Harmful to invertebrates (Daphnia). Not harmful to algae (EC50 >1000 mg/l). Not harmful to plankton. According to literature: harmful to the activated sludge.

acetone-D6 (666-52-4)	
LC50 fishes 1	5540 mg/l (96 hours; SALMO GAIRDNERI/ ONCORHYNCHUS MYKISS; NON DEUTERIUM FORM)
LC50 other aquatic organisms 1	10 mg/l (48 hours; DAPHNIA MAGNA; NON DEUTERIUM FORM)
EC50 Daphnia 1	39 mg/l (48 hours; DAPHNIA MAGNA; NON DEUTERIUM FORM)
EC50 other aquatic organisms 1	1700 mg/l (PSEUDOMONAS PUTIDA; NON DEUTERIUM FORM)
LC50 fishes 2	6210 mg/l (96 hours; PIMEPHALES PROMELAS; NON DEUTERIUM FORM)
LC50 other aquatic organisms 2	2100 mg/l (48 hours; ARTEMIA SALINA; NON DEUTERIUM FORM)
EC50 Daphnia 2	8800 mg/l (48 hours; DAPHNIA PULEX; NON DEUTERIUM FORM)
EC50 other aquatic organisms 2	> 7000 mg/l (96 hours; SELENASTRUM CAPRICORNUTUM; NON DEUTERIUM FORM)

12.2. Persistence and degradability

acetone-D6 (666-52-4)	
Persistence and degradability	Literature reports: nitrification is inhibited. Readily biodegradable in water. test: 81 %, OECD 302B Zahn-Well . test: 0%, 28d, mitil, OECD 301C . According to literature, degradable in the soil. According to literature, degradable in the soil in anaerobic conditions.
Biochemical oxygen demand (BOD)	1.43 g O ₂ /g substance
Chemical oxygen demand (COD)	1.92 g O ₂ /g substance
ThOD	2.20 g O ₂ /g substance
BOD (% of ThOD)	65 % ThOD

12.3. Bioaccumulative potential

acetone-D6 (666-52-4)	
BCF fishes 2	0.69 (PISCES; NON DEUTERIUM FORM)
Log Pow	-0.24 (exp.)
Bioaccumulative potential	Bioaccumulation: not applicable.

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

No additional information available

acetone-D6

Safety Data Sheet

according to Regulation (EC) No. 453/2010

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste disposal recommendations : Remove waste in accordance with local and/or national regulations. Recycle by distillation. Remove to an authorized waste incinerator for solvents with energy recovery. Do not discharge into surface water.

Additional information : LWCA (the Netherlands): KGA category 03. Hazardous waste (91/689/EEC).

SECTION 14: Transport information

In accordance with ADR / RID / ADNR / IMDG / ICAO / IATA

14.1. UN number

UN-No. : 1090

14.2. UN proper shipping name

Transport document description : UN 1090, 3, II, (D/E)

14.3. Transport hazard class(es)

Class (UN) : 3

Hazard labels (UN) : 3



14.4. Packing group

Packing group (UN) : II

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

14.6.1. Overland transport

Hazard identification number (Kemler No.) : 33

Classification code : F1

Orange plates : 

Tunnel restriction code : D/E

EAC code : •2YE

14.6.2. Transport by sea

EmS-No. (1) : F-E

EmS-No. (2) : S-D

14.6.3. Air transport

Instruction "cargo" (ICAO) : 307

Instruction "passenger" (ICAO) : 305

Instruction "passenger" - Limited quantities (ICAO) : Y305

14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

IBC code : IBC02.

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

VOC content : 100 %

EURAL code : 07 01 04*

15.1.2. National regulations

No additional information available

15.2. Chemical safety assessment

No additional information available

acetone-D6

Safety Data Sheet

according to Regulation (EC) No. 453/2010

SECTION 16: Other information

Full text of R-, H- and EUH-phrases:

Eye Irrit. 2	Serious eye damage/eye irritation Category 2
Flam. Liq. 2	Flammable liquids Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H225	Highly flammable liquid and vapour
H319	Causes serious eye irritation
H336	May cause drowsiness or dizziness
R11	Highly flammable.
R36	Irritating to eyes.
R66	Repeated exposure may cause skin dryness or cracking.
R67	Vapours may cause drowsiness and dizziness.

SDS EU (REACH Annex II)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

