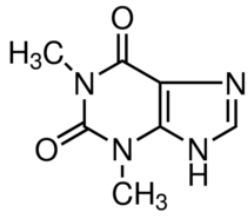
THEOPHYLLINE ANHYDROUS EXTRA PURE

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878
SDS Reference Number: 06254
Issue date: 4/9/2014 Revision date: 9/2/2026 Supersedes version of: 4/9/2015 Version: 1.0

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

1.1. Product identifier

Product form	:	Substance
Trade name	:	THEOPHYLLINE ANHYDROUS EXTRA PURE
IUPAC name	:	3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione
EC Index-No.	:	613-342-00-6
EC-No.	:	200-385-7
CAS-No.	:	58-59-5
Product code	:	06254
Type of product	:	Heterocyclic organic compound
Formula	:	C7H8N4O2
Chemical structure	:	
Synonyms	:	1,3-Dimethyl xanthine, 2,6-Dihydroxy-1,3-dimethylpurine

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

Relevant identified uses

Use of the substance/mixture	:	Laboratory chemicals, Manufacture of substances

1.3. Details of the supplier of the safety data sheet

LOBA CHEMIE PVT.LTD.
107 Wode House Road, Jehangir Villa, Colaba
400005 Mumbai
INDIA
T +91 22 6663 6663, F +91 22 6663 6699
info@lobachemie.com, www.lobachemie.com

1.4. Emergency telephone number

Emergency number	:	+ 91 22 6663 6663 (9:00am - 6:00 pm)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

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

Acute toxicity (oral), Category 3	H301
Reproductive toxicity, Category 1B	H360D

Full text of H- and EUH-statements: see section 16

Adverse physicochemical, human health and environmental effects

May damage the unborn child. Toxic if swallowed.

2.2. Label elements

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

Hazard pictograms (CLP) :



GHS06 GHS08

Signal word (CLP) : Danger

Hazard statements (CLP) : H301 - Toxic if swallowed.
H360D - May damage the unborn child.

Precautionary statements (CLP) : P202 - Do not handle until all safety precautions have been read and understood.
P264 - Wash hands and forearms thoroughly after handling.
P280 - Wear respiratory protection, protective gloves, protective clothing, eye protection.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor.

2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%
THEOPHYLLINE ANHYDROUS	CAS-No.: 58-59-5 EC-No.: 200-385-7 EC Index-No.: 613-342-00-6	100

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : Call a physician immediately.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. Give oxygen or artificial respiration if necessary.

First-aid measures after skin contact : Gently wash with plenty of soap and water. If skin irritation occurs: Get medical advice/attention. Wash skin with plenty of water.

First-aid measures after eye contact : Remove contact lenses, if present and easy to do. Continue rinsing. Rinse cautiously with water for several minutes. If eye irritation persists: Get medical advice/attention.

First-aid measures after ingestion : Rinse mouth. Call a POISON CENTER/doctor if you feel unwell. Call a physician immediately.

Self protection of the first-aider : First-aiders should pay attention to their own protection and use the recommended personal protective equipment (see section 8).

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

Symptoms/effects after inhalation : None under normal conditions. Dust of the product, if present, may cause respiratory irritation after excessive inhalation exposure.

Symptoms/effects after skin contact : None under normal conditions. Dust may cause irritation in skin folds or by contact in combination with tight clothing.

Symptoms/effects after eye contact : None under normal conditions. Dust from this product may cause eye irritation.

Symptoms/effects after ingestion : Toxic if swallowed.

Chronic symptoms : May damage the unborn child.

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

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : dry chemical powder, alcohol-resistant foam, carbon dioxide (CO2). Water spray. Dry powder. Foam.

Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Fire hazard : No fire hazard.
Explosion hazard : No direct explosion hazard.
Hazardous decomposition products in case of fire : Toxic fumes may be released.

5.3. Advice for firefighters

Firefighting instructions : Fight fire from safe distance and protected location. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Notify authorities if product enters sewers or public waters. Absorb spillage to prevent material damage.

For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.
Emergency procedures : Evacuate unnecessary personnel. Only qualified personnel equipped with suitable protective equipment may intervene.

For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Use personal protective equipment as required. For further information refer to section 8: "Exposure controls/personal protection".
Emergency procedures : Stop release. Evacuate unnecessary personnel.

6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

For containment : Using a clean shovel, put the material in a dry container and cover without compressing it.
Methods for cleaning up : Mechanically recover the product. Clear up rapidly by scoop or vacuum. Notify authorities if product enters sewers or public waters.
Other information : Dispose of materials or solid residues at an authorized site.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Not expected to present a significant hazard under anticipated conditions of normal use.
Precautions for safe handling : Ensure good ventilation of the work station. Do not get in eyes, on skin, or on clothing. Obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Wear personal protective equipment.
Hygiene measures : Do not eat, drink or smoke when using this product. Wash hands, forearms and face thoroughly after handling. Separate working clothes from town clothes. Launder separately. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Keep in a cool, well-ventilated place away from heat.
Storage conditions : Store in original container. Keep container tightly closed. Store in a dry place. Protect from moisture. Store locked up.

Packaging materials : Always store product in container of same material as original container.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls

Appropriate engineering controls:
Ensure good ventilation of the work station.

Personal protection equipment

Personal protective equipment:
Wear recommended personal protective equipment.
Personal protective equipment symbol(s):



Eye and face protection

Eye protection:
Chemical goggles or safety glasses

Skin protection

Skin and body protection:
Wear a mask

Hand protection:
Protective gloves

Respiratory protection

Respiratory protection:
Wear appropriate mask. [In case of inadequate ventilation] wear respiratory protection.

Environmental exposure controls

Environmental exposure controls:
Avoid release to the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	:	Solid
Colour	:	White.
Appearance	:	Crystalline powder.
Molecular mass	:	180.17 g/mol
Odour	:	Odourless.
Odour threshold	:	Not available
Melting point	:	271 – 273 °C
Freezing point	:	Not applicable
Boiling point	:	Not available
Flammability	:	Non flammable
Lower explosion limit	:	Not applicable
Upper explosion limit	:	Not applicable

Flash point	:	Not applicable
Auto-ignition temperature	:	Not applicable
Decomposition temperature	:	Not available
pH	:	5
pH solution concentration	:	8 g/L
Viscosity, kinematic	:	Not applicable
Solubility	:	Water: 8.3 g/l at 20 °C - Slightly soluble in water Ethanol: Slightly soluble in Ethanol Ether: Slightly soluble in Ether
Partition coefficient n-octanol/water (Log Kow)	:	Not available
Partition coefficient n-octanol/water (Log Pow)	:	-0.008 at 23 °C
Vapour pressure	:	Negligible
Vapour pressure at 50°C	:	Not available
Density	:	1.36 g/cm³ at 25 °C
Relative density	:	Not available
Relative vapour density at 20°C	:	Not applicable
Particle size	:	Not available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Direct sunlight. Air contact. Moisture.

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity (oral)	:	Toxic if swallowed.
Acute toxicity (dermal)	:	Not classified
Acute toxicity (inhalation)	:	Not classified
Skin corrosion/irritation	:	Not classified pH: 5
Serious eye damage/irritation	:	Not classified pH: 5
Respiratory or skin sensitisation	:	Not classified
Germ cell mutagenicity	:	Not classified
Carcinogenicity	:	Not classified
Reproductive toxicity	:	May damage the unborn child.
STOT-single exposure	:	Not classified

STOT-repeated exposure : Not classified
Aspiration hazard : Not classified

THEOPHYLLINE ANHYDROUS EXTRA PURE (58-59-5)	
Viscosity, kinematic	Not applicable

11.2. Information on other hazards

Other information

Potential adverse human health effects and symptoms : Harmful if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms nor to cause long-term adverse effects in the environment.
Hazardous to the aquatic environment, short–term (acute) : Not classified
Hazardous to the aquatic environment, long–term (chronic) : Not classified

12.2. Persistence and degradability

THEOPHYLLINE ANHYDROUS EXTRA PURE (58-59-5)	
Persistence and degradability	Rapidly degradable

12.3. Bioaccumulative potential

THEOPHYLLINE ANHYDROUS EXTRA PURE (58-59-5)	
Partition coefficient n-octanol/water (Log Pow)	-0.008 at 23 °C

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Endocrine disrupting properties

No additional information available

12.7. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional waste regulation : Disposal must be done according to official regulations.
Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.
Sewage disposal recommendations : Disposal must be done according to official regulations.
Product/Packaging disposal recommendations : Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation. Disposal must be done according to official regulations.
Additional information : Do not re-use empty containers.

Ecological waste information	:	The waste of the product should be considered as hazardous as the product itself, with the likelihood of impacting the environment in the same way. Consider the handling and disposal of the waste as defined by the product itself.

SECTION 14: Transport information

In accordance with ADR / IMDG / IATA / ADN / RID

14.1. UN number or ID number

UN-No. (ADR)	:	UN 2811
UN-No. (IMDG)	:	UN 2811
UN-No. (IATA)	:	UN 2811
UN-No. (ADN)	:	UN 2811
UN-No. (RID)	:	UN 2811

14.2. UN proper shipping name

Proper Shipping Name (ADR)	:	TOXIC SOLID, ORGANIC, N.O.S.
Proper Shipping Name (IMDG)	:	TOXIC SOLID, ORGANIC, N.O.S.
Proper Shipping Name (IATA)	:	Toxic solid, organic, n.o.s.
Proper Shipping Name (ADN)	:	TOXIC SOLID, ORGANIC, N.O.S.
Proper Shipping Name (RID)	:	TOXIC SOLID, ORGANIC, N.O.S.
Transport document description (ADR) (ADR)	:	UN 2811 TOXIC SOLID, ORGANIC, N.O.S. THEOPHYLLINE ANHYDROUS, 6.1, III, (E)
Transport document description (IMDG)	:	UN 2811 TOXIC SOLID, ORGANIC, N.O.S., 6.1, III
Transport document description (IATA)	:	UN 2811 Toxic solid, organic, n.o.s. THEOPHYLLINE ANHYDROUS, 6.1, III
Transport document description (ADN)	:	UN 2811 TOXIC SOLID, ORGANIC, N.O.S., 6.1, III
Transport document description (RID)	:	UN 2811 TOXIC SOLID, ORGANIC, N.O.S., 6.1, III

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR) : 6.1

Danger labels (ADR) : 6.1

:



IMDG

Transport hazard class(es) (IMDG) : 6.1

Danger labels (IMDG) : 6.1

:



IATA

Transport hazard class(es) (IATA) : 6.1

Danger labels (IATA) : 6.1

:



ADN

Transport hazard class(es) (ADN) : 6.1

Danger labels (ADN) : 6.1

:



RID

Transport hazard class(es) (RID) : 6.1

Danger labels (RID) : 6.1

:



14.4. Packing group

Packing group (ADR) : III

Packing group (IMDG) : III

Packing group (IATA) : III

Packing group (ADN) : III

Packing group (RID) : III

14.5. Environmental hazards

Dangerous for the environment : No

Marine pollutant : No

EmS-No. (Fire) : F-A

EmS-No. (Spillage) : S-A

Other information : No supplementary information available

14.6. Special precautions for user

Overland transport

Classification code (ADR) : T2

Special provisions (ADR) : 274, 614

Limited quantities (ADR) : 5kg

Excepted quantities (ADR) : E1

Packing instructions (ADR) : P002, IBC08, LP02, R001

Special packing provisions (ADR) : B3

Mixed packing provisions (ADR) : MP10

Portable tank and bulk container instructions (ADR) : T1

Portable tank and bulk container special provisions (ADR) : TP33

Tank code (ADR) : SGAH, L4BH

Tank special provisions (ADR) : TU15, TE19

Vehicle for tank carriage : AT

Transport category (ADR) : 2

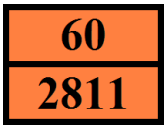
Special provisions for carriage - Bulk (ADR) : VC1, VC2, AP7

Special provisions for carriage - Loading, unloading and handling (ADR) : CV13, CV28

Special provisions for carriage - Operation (ADR) : S9

Hazard identification number (Kemler No.) : 60

Orange plates :



Tunnel restriction code (ADR) : E

EAC code : 2X

Transport by sea

Special provisions (IMDG) : 223, 274

Limited quantities (IMDG) : 5 kg

Excepted quantities (IMDG) : E1

Packing instructions (IMDG) : P002

IBC packing instructions (IMDG)	:	IBC08
IBC special provisions (IMDG)	:	B3
Tank instructions (IMDG)	:	T1
Tank special provisions (IMDG)	:	TP33
Stowage category (IMDG)	:	A
Properties and observations (IMDG)	:	Toxic if swallowed, by skin contact or by inhalation.
MFAG-No	:	154

Air transport

PCA Excepted quantities (IATA)	:	E1
PCA Limited quantities (IATA)	:	Y645
PCA limited quantity max net quantity (IATA)	:	10kg
PCA packing instructions (IATA)	:	670
PCA max net quantity (IATA)	:	100kg
CAO packing instructions (IATA)	:	677
CAO max net quantity (IATA)	:	200kg
Special provisions (IATA)	:	A3, A5
ERG code (IATA)	:	6L

Inland waterway transport

Classification code (ADN)	:	T2
Special provisions (ADN)	:	274, 614, 802
Limited quantities (ADN)	:	5 kg
Excepted quantities (ADN)	:	E1
Carriage permitted (ADN)	:	T
Equipment required (ADN)	:	PP, EP
Number of blue cones/lights (ADN)	:	0

Rail transport

Classification code (RID)	:	T2
Special provisions (RID)	:	274, 614
Limited quantities (RID)	:	5kg
Excepted quantities (RID)	:	E1
Packing instructions (RID)	:	P002, IBC08, LP02, R001
Special packing provisions (RID)	:	B3
Mixed packing provisions (RID)	:	MP10
Portable tank and bulk container instructions (RID)	:	T1
Portable tank and bulk container special provisions (RID)	:	TP33
Tank codes for RID tanks (RID)	:	SGAH, L4BH
Special provisions for RID tanks (RID)	:	TU15
Transport category (RID)	:	2
Special provisions for carriage – Bulk (RID)	:	VC1, VC2, AP7
Special provisions for carriage - Loading, unloading and handling (RID)	:	CW13, CW28, CW31
Colis express (express parcels) (RID)	:	CE11
Hazard identification number (RID)	:	60

14.7. Maritime transport in bulk according to IMO instruments

Not applicable

SECTION 15: Regulatory information

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

EU-Regulations

REACH Annex XVII (Restriction List)

Not listed on REACH Annex XVII

REACH Annex XIV (Authorisation List)

Not listed on REACH Annex XIV (Authorisation List)

REACH Candidate List (SVHC)

Not listed on the REACH Candidate List

PIC Regulation (Prior Informed Consent)

Not listed on the PIC list (Regulation EU 649/2012)

POP Regulation (Persistent Organic Pollutants)

Not listed on the POP list (Regulation EU 2019/1021)

Ozone Regulation (2024/590)

Not listed on the Ozone Depletion list (Regulation EU 2024/590)

Council Regulation (EC) for the control of dual-use items

Not listed on the COUNCIL REGULATION (EC) of dual-use items.

Explosives Precursors Regulation (EU 2019/1148)

Not listed on the Explosives Precursors list (EU)

Drug Precursors Regulation (EC 273/2004)

Not listed on the Drug Precursors list (EU)

National regulations

Denmark

Danish National Regulations	:	Young people below the age of 18 years are not allowed to use the product Pregnant/breastfeeding women working with the product must not be in direct contact with it. If an employee is pregnant or breastfeeding and the person in question uses or is exposed to this product at work, the employer must always carry out a risk assessment of the work. The assessment must both deal with the dangerousness of the impact and its strength and duration. The employer's decision that a pregnant or lactating woman can perform a specific work task must therefore be made in the context of her specific working conditions. See also WEA-Guideline A.1.8-7 on the working environment of pregnant and breastfeeding workers. The requirements from the Danish Working Environment Authorities regarding work with carcinogens must be followed during use and disposal

Germany

Water hazard class (WGK)	:	WGK 1, Slightly hazardous to water (Classification according to AwSV; ID No. 8278).
Chemicals Prohibition Ordinance (ChemVerbotsV)	:	This product is subject to ChemVerbotsV Annex 2 Entry 1. The following requirements must be observed: authorization requirement (according to § 6 paragraph 1 sentence 1), basic requirements for carrying out the delivery (according to § 8 paragraph 1, 3 and 4), identification and documentation (according to § 9 paragraph 1 to 3) and exclusion of the shipping route (according to § 10).

Netherlands

SZW List of Carcinogenic Substances	:	The substance is not listed
SZW List of Mutagenic Substances	:	The substance is not listed
SZW List of Reprotoxic Substances – Breastfeeding	:	The substance is not listed
SZW List of Reprotoxic Substances – Fertility	:	The substance is not listed
SZW List of Reprotoxic Substances – Development	:	The substance is not listed

Poland

Polish National Regulations : Act of 25 February 2011 on chemical substances and their mixtures (J. o L. No. 63, item 322 as amended; consolidated text J. o L. 2019, item 1225).
Act of 14 December 2012 on waste (J. o L. 2013, item 322 as amended; consolidated text J. o L. 2020, item 797).
The announcement of Marshal of the Sejm of the Republic of Poland dated 19 October 2016 concerning the consolidated text announcement of the decree on the management of packaging and packaging waste (J. o L. 2016, item 1863 as amended).
Decree of the Minister of Environment of 14 December 2014 on the catalogue of waste (J. o L. 2014, item 1923).
Act of 19 August 2011 on the Carriage of Dangerous Goods (J. o L. 2011 No. 227, item 1367 as amended; consolidated text J. o L. 2020, item 154).
Regulation of the Minister of Family, Labour and Social Policy of 12 June 2018 on the highest permissible concentration and intensity of noxious agents for health at work environment (J. o L. item 1286 as amended).
The announcement of Minister of Health dated 9 September 2016 concerning the consolidated text announcement of the decree of the Minister of Health of 30 December 2004 on health and safety at work related to exposure to chemical agents at work (J. o L. of 16 September 2016, item 1488)
Regulation of the Minister of Health of 2 February 2011 on tests and measurements of the noxious agents for health at work environment (J. o L. No. 33, item 166 as amended).
Regulation of the Minister of Environment of 9 December 2003 on particularly hazardous substances to the environment (J. o L. No. 217, item 2141).
ADR Agreement: Government Statement of 13 March 2023 on the entry into force of amendments to Annexes A and B to the Agreement concerning the International Carriage of Dangerous Goods by Road (ADR), signed in Geneva on 30 September 1957 (J. o. L. 2023, item 891)
Regulation of the Minister of Health of 25 August 2015 on the method of marking places, pipelines, and containers and tanks used for storing or containing hazardous substances or hazardous mixtures (J.o.L. 2015, item 1368 as amended)

15.2. Chemical safety assessment

No chemical safety assessment has been carried out

SECTION 16: Other information

Abbreviations and acronyms:	
ACGIH	American Conference of Governmental Industrial Hygienists
ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
BLV	Biological limit value
BOD	Biochemical oxygen demand (BOD)
CAS-No.	Chemical Abstracts Service number
CLP	Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008
COD	Chemical oxygen demand (COD)
CSA	Chemical safety assessment
DMEL	Derived Minimal Effect level
DNEL	Derived-No Effect Level
EC-No.	European Community number

Abbreviations and acronyms:	
EC50	Median effective concentration
ED	Endocrine disruptor
EN	European Standard
EWC	European waste catalogue
IARC	International Agency for Research on Cancer
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods
LC50	Median lethal concentration
LD50	Median lethal dose
LOAEL	Lowest Observed Adverse Effect Level
Log Kow	Partition coefficient n-octanol/water (Log Kow)
Log Pow	Partition coefficient n-octanol/water (Log Pow)
MAK	maximum workplace concentration
NOAEC	No-Observed Adverse Effect Concentration
NOAEL	No-Observed Adverse Effect Level
NOEC	No-Observed Effect Concentration
N.O.S.	Not Otherwise Specified
OECD	Organisation for Economic Co-operation and Development
OEL	Occupational Exposure Limit
OSHA	Occupational Safety & Health Administration
PBT	Persistent Bioaccumulative Toxic
PNEC	Predicted No-Effect Concentration
PPE	Personal protection equipment
RID	Regulations concerning the International Carriage of Dangerous Goods by Rail
SDS	Safety Data Sheet
STP	Sewage treatment plant
TF	Technical function
ThOD	Theoretical oxygen demand (ThOD)
TLM	Median Tolerance Limit
TWA	Time Weighted Average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and Very Bioaccumulative
UFI	Unique Formula Identifier

Full text of H- and EUH-statements:	
Acute Tox. 3 (Oral)	Acute toxicity (oral), Category 3
Repr. 1B	Reproductive toxicity, Category 1B
H301	Toxic if swallowed.
H360D	May damage the unborn child.

Safety Data Sheet (SDS), EU

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.