

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Chloral hydrate ≥98 %, for synthesis

article number: **1HH6**
Version: **1.0 en**

date of compilation: 2021-03-03

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

1.1 Product identifier

Identification of the substance	Chloral hydrate ≥98 %, for synthesis
Article number	1HH6
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
Index number in CLP Annex VI	605-014-00-6
EC number	206-117-5
CAS number	302-17-0
Alternative name(s)	2,2,2-trichloroethane-1,1-diol

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household).

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

Telephone: +49 (0) 721 - 56 06 0
Telefax: +49 (0) 721 - 56 06 149
e-mail: sicherheit@carlroth.de
Website: www.carlroth.de

Competent person responsible for the safety data sheet: :Department Health, Safety and Environment

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

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SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.10	Acute toxicity (oral)	3	Acute Tox. 3	H301
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315
3.3	Serious eye damage/eye irritation	2	Eye Irrit. 2	H319

For full text of abbreviations: see SECTION 16

2.2 Label elements

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

Signal word **Danger**

Pictograms

GHS06



Hazard statements

H301 Toxic if swallowed
H315 Causes skin irritation
H319 Causes serious eye irritation

Precautionary statements

Precautionary statements - prevention

P270 Do not eat, drink or smoke when using this product
P280 Wear protective gloves/eye protection

Precautionary statements - response

P302+P352 IF ON SKIN: Wash with plenty of 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

Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H301 Toxic if swallowed.
P270 Do not eat, drink or smoke when using this product.

2.3 Other hazards

This material is combustible, but will not ignite readily.

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Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Chloral hydrate
Molecular formula	$C_2H_3Cl_3O_2$
Molar mass	165,4 g/mol
CAS No	302-17-0
EC No	206-117-5
Index No	605-014-00-6

Specific Conc. Limits	M-Factors	ATE	Exposure route
		100 mg/kg	oral

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

Breathing difficulties, Unconsciousness, Vomiting, Nausea, Irritation

4.3 Indication of any immediate medical attention and special treatment needed

Give sodium sulfate as laxative (1 tablespoon in 1 glass of water).

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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings
water, foam, alcohol resistant foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen chloride (HCl)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe dust.

6.2 Environmental precautions

Keep away from drains, surface and ground water.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Use extractor hood (laboratory). Avoid dust formation. Clear contaminated areas thoroughly.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Advice on general occupational hygiene

When using do not eat or drink. Thorough skin-cleansing after handling the product.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

Store locked up.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Data are not available.

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	1,716 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	0,973 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

Environmental values

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Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,115 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,011 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	7,9 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,09 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,009 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,02 mg/kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 °C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

NBR (Nitrile rubber)

• material thickness

>0,11 mm

• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

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Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P3 (filters at least 99,95 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	solid
Form	crystalline
Colour	white
Odour	stinging
Melting point/freezing point	52 °C
Boiling point or initial boiling point and boiling range	97 °C at 1.013 hPa (slow decomposition)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	75 °C at 973,4 hPa (ECHA)
Auto-ignition temperature	not determined
Decomposition temperature	>97 °C
pH (value)	3,5 – 5,5 (in aqueous solution: 100 g/l, 20 °C)
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	~ 6.600 g/l at 20 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	1,092 (25 °C) (ECHA)
Soil organic carbon/water (log KOC)	0,217 (ECHA)
Vapour pressure	13 hPa at 20 °C
Density	1,91 g/cm ³ at 20 °C
Relative vapour density	5,7 (air = 1)

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Particle characteristics no data available

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard classes: hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics: There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser, Alkali metals, Alcohols, Bases, Alkaline earth metal, Permanganates

10.4 Conditions to avoid

Keep away from heat. Decomposition takes place from temperatures above: $>97\text{ }^{\circ}\text{C}$.

10.5 Incompatible materials

iron, different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

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

Classification according to GHS (1272/2008/EC, CLP)

Acute toxicity

Toxic if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	479 mg/kg	rat		TOXNET
dermal	LD50	3.030 mg/kg	rat		TOXNET

Skin corrosion/irritation

Causes skin irritation.

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Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

vomiting, nausea

• If in eyes

Causes serious eye irritation

• If inhaled

Inhalation of dust may cause irritation of the respiratory system

• If on skin

causes skin irritation

• Other information

Other adverse effects: Liver and kidney damage, Cardiac arrhythmias, Dyspnoea, Blood pressure drop, Unconsciousness, Drowsiness

11.2 Endocrine disrupting properties

Not listed.

11.3 Information on other hazards

There is no additional information.

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SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)			
Endpoint	Value	Species	Exposure time
LC50	>100 mg/l	fish	96 h

Aquatic toxicity (chronic)			
Endpoint	Value	Species	Exposure time
EC50	65 mg/l	aquatic invertebrates	21 d

Biodegradation

Data are not available.

12.2 Process of degradability

Theoretical Oxygen Demand: 0,1935 mg/mg
Theoretical Carbon Dioxide: 0,5322 mg/mg

Process of degradability		
Process	Degradation rate	Time
biotic/abiotic	4 %	14 d
oxygen depletion	44,04 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1,092 (25 °C) (ECHA)
BCF	3,162 (ECHA)

12.4 Mobility in soil

Henry's law constant	0 Pa m ³ /mol at 25 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	0,217 (ECHA)

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 Other adverse effects

Data are not available.

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SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process. Waste catalogue ordinance (Germany).

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

SECTION 14: Transport information

14.1 UN number or ID number

ADR/RID/ADN	UN 2811
IMDG-Code	UN 2811
ICAO-TI	UN 2811

14.2 UN proper shipping name

ADR/RID/ADN	TOXIC SOLID, ORGANIC, N.O.S.
IMDG-Code	TOXIC SOLID, ORGANIC, N.O.S.
ICAO-TI	Toxic solid, organic, n.o.s.
Technical name	Chloral hydrate

14.3 Transport hazard class(es)

ADR/RID/ADN	6.1
IMDG-Code	6.1
ICAO-TI	6.1

14.4 Packing group

ADR/RID/ADN	III
IMDG-Code	III
ICAO-TI	III

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

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14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

Information for each of the UN Model Regulations

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information

Classification code	T2
Danger label(s)	6.1
Special provisions (SP)	274, 614, 802(ADN)
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
Transport category (TC)	2
Tunnel restriction code (TRC)	E
Hazard identification No	60
Emergency Action Code	2X

International Maritime Dangerous Goods Code (IMDG) - Additional information

Marine pollutant	-
Danger label(s)	6.1
Special provisions (SP)	223, 274
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 kg
EmS	F-A, S-A
Stowage category	A

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Danger label(s)	6.1
Special provisions (SP)	A3, A5
Excepted quantities (EQ)	E1
Limited quantities (LQ)	10 kg

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SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

Not listed.

Seveso Directive

2012/18/EU (Seveso III)			
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
	not assigned		

Deco-Paint Directive (2004/42/EC)

VOC content	100 % 1.910 g/l
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Directive on industrial emissions (VOCs, 2010/75/EU)

VOC content	100 %
VOC content	1.910 g/l

Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

List of pollutants (WFD)				
Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
Chloral hydrate	Organohalogen compounds and substances which may form such compounds in the aquatic environment		A)	
Chloral hydrate	Substances and preparations, or the breakdown products of such, which have been proved to possess carcinogenic or mutagenic properties or properties which may affect steroidogenic, thyroid, reproduction or other endocrine-related functions in or via the aquatic environment		A)	

Legend

A) Indicative list of the main pollutants

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Regulation 98/2013/EU on the marketing and use of explosives precursors

not listed

Regulation 111/2005/EC laying down rules for the monitoring of trade between the Community and third countries in drug precursors

not listed

Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)

not listed

Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)

not listed

National inventories

Country	Inventory	Status
AU	AICS	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed

Legend

AICS	Australian Inventory of Chemical Substances
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

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SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
ADR/RID/ADN	European Agreements concerning the International Carriage of Dangerous Goods by Road/Rail/Inland Waterways (ADR/RID/ADN)
ATE	Acute Toxicity Estimate
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
index No	The Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

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Abbr.	Descriptions of used abbreviations
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
H301	Toxic if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.