

P-Chlorobenzotrifluoride (PCBTF)

Version number: 3.0

SECTION 1: Identification

1.1 Product identifier

Identification of the substance	4-chlorbenzotrifluoride
Trade name	<u>P-Chlorobenzotrifluoride (PCBTF)</u>
CAS number	98-56-6

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

Relevant identified uses	Chemicals for various applications Intermediate Solvent Use in Coatings Intermediate for organic synthesis
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1.3 Details of the supplier of the safety data sheet

Valudor Products, LLC 179 Calle Magdalena Suite 100 Encinitas, California CA 92024 United States	Telephone: +1 (760) 635 8500 e-mail: info@valudor.com Website: www.valudor.com
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1.4 Emergency telephone number

Emergency information	800-535-5053 (Infotrac)
As above or nearest toxicological information center.	

SECTION 2: Hazard(s) identification

2.1 Classification of the substance or mixture

Classification acc. to OSHA "Hazard Communication Standard" (29 CFR 1910.1200)

Classification				
Section	Hazard class	Category	Hazard class and category	Hazard statement
A.4S	skin sensitization	1B	Skin Sens. 1B	H317
A.6	carcinogenicity	2	Carc. 2	H351
A.7	reproductive toxicity	2	Repr. 2	H361
B.6	flammable liquid	3	Flam. Liq. 3	H226

For full text of abbreviations: see SECTION 16

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The most important adverse physicochemical, human health and environmental effects

The product is combustibile and can be ignited by potential ignition sources.

2.2 Label elements

Labelling acc. to OSHA "Hazard Communication Standard" (29 CFR 1910.1200)

Signal word warning

Pictograms

GHS02, GHS07, GHS08



Hazard statements

H226	Flammable liquid and vapor.
H317	May cause an allergic skin reaction.
H351	Suspected of causing cancer (if inhaled).
H361	Suspected of damaging fertility or the unborn child (if inhaled).

Precautionary statements

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ventilating/lighting/tooling equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing mist/vapors/spray.
P272	Contaminated work clothing must not be allowed out of the workplace.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352	IF ON SKIN: Wash with plenty of soap and water.
P303+P361+P353	If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P308+P313	If exposed or concerned: Get medical advice/attention.
P363	Wash contaminated clothing before reuse.
P370+P378	In case of fire: Use carbon dioxide, powder extinguisher or water spray to extinguish.
P403+P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3 Other hazards

Results of PBT and vPvB assessment

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

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	4-chlorbenzotrifluoride
Identifiers	
CAS No	98-56-6
Molecular formula	C ₇ H ₄ ClF ₃
Molar mass	180.6 g/mol
Purity	≥ 99.5 %

SECTION 4: First-aid measures

4.1 Description of first-aid measures

General notes

Self-protection of the first aider.

Remove affected person from the danger area and lay down.

Do not leave affected person unattended.

Take off immediately all contaminated clothing.

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

Following inhalation

Provide fresh air.

Mouth to mouth resuscitation should be avoided. Use alternative methods, preferably with oxygen or compressed air driven apparatus.

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions.

Keep affected person warm, still and covered.

Following skin contact

After contact with skin, take off immediately all contaminated clothing, and wash immediately with plenty of water and soap.

If skin irritation or rash occurs: Get medical advice/attention.

Wash contaminated clothing before reuse.

Following eye contact

In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

Remove contact lenses, if present and easy to do. Continue rinsing.

Following ingestion

Rinse mouth immediately and drink plenty of water.

Do NOT induce vomiting.

In case of unconsciousness place person in the recovery position. Never give anything by mouth.

Get medical advice/attention.

Notes for the doctor

None.

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4.2 Most important symptoms and effects, both acute and delayed

Toxic effects for reproduction.
Cough.
Irritant effects.

4.3 Indication of any immediate medical attention and special treatment needed

None.

SECTION 5: Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

water spray, alcohol resistant foam, fire extinguishing powder, carbon dioxide (CO₂), sand

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous decomposition products: Section 10.

In case of insufficient ventilation and/or in use, may form flammable/explosive vapor-air mixture.

Solvent vapors are heavier than air and may spread along floors.

Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures.

Hazardous combustion products

carbon monoxide (CO), carbon dioxide (CO₂), hydrogen chloride (HCl), hydrogen fluoride (HF), toxic gases/vapours

5.3 Advice for firefighters

Keep containers cool with water spray.

In case of fire and/or explosion do not breathe fumes.

Coordinate firefighting measures to the fire surroundings.

Do not allow firefighting water to enter drains or water courses.

Collect contaminated firefighting water separately.

Fight fire with normal precautions from a reasonable distance.

Special protective equipment for firefighters

chemical protection suit, self-contained breathing apparatus (SCBA)

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Keep away from sources of ignition - No smoking.

Remove persons to safety.

Ventilate affected area.

Do not breathe mist/vapors/spray.

Do not get in eyes, on skin, or on clothing.

Wearing of suitable protective equipment (including personal protective equipment referred to under

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Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing.

For emergency responders

Wear breathing apparatus if exposed to vapors/dust/aerosols/gases.

6.2 Environmental precautions

Keep away from drains, surface and ground water.

Retain contaminated washing water and dispose of it.

If substance has entered a water course or sewer, inform the responsible authority.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Set up barriers.

Covering of drains.

Advice on how to clean up a spill

Collect spillage.

Absorbent material (e.g. sand, diatomaceous earth, acid binder, universal binder, sawdust, etc.).

Appropriate containment techniques

Use of adsorbent materials.

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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Obtain special instructions before use.

Measures to prevent fire as well as aerosol and dust generation

Use local and general ventilation.

Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge.

Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches.

Ground/bond container and receiving equipment.

Use explosion-proof electrical/ventilating/lighting/equipment.

Use only non-sparking tools.

Specific notes/details

Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures.

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

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Measures to protect the environment

Avoid release to the environment.

Do not empty into drains; dispose of this material and its container at hazardous or special waste collection point.

Advice on general occupational hygiene

Do not eat, drink and smoke in work areas.

Remove contaminated clothing and protective equipment before entering eating areas.

Do not breathe mist/vapors/spray.

Do not get in eyes, on skin, or on clothing.

Avoid contact during pregnancy/while nursing.

Wash thoroughly after handling.

Preventive skin protection (barrier creams/ointments) is recommended.

7.2 Conditions for safe storage, including any incompatibilities

Explosive atmospheres

Keep container tightly closed and in a well-ventilated place.

Use local and general ventilation.

Keep cool.

Protect from sunlight.

Flammability hazards

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Take precautionary measures against static discharge.

Ground/bond container and receiving equipment.

Protect from sunlight.

Incompatible substances or mixtures

Incompatible materials: see section 10.

Protect against external exposure, such as

heat, humidity

Consideration of other advice

Keep away from food, drink and animal feedingstuffs.

Ventilation requirements

Provision of sufficient ventilation.

Specific designs for storage rooms or vessels

Keep container tightly closed and in a well-ventilated place.

Keep cool.

Store in a dry place.

Packaging compatibilities

Only packagings which are approved (e.g. acc. to DOT) may be used.

7.3 Specific end use(s)

No information available.

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SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limit values (Workplace Exposure Limits)

No constituent of the product currently has a known exposure limit.

8.2 Exposure controls

Avoid contact during pregnancy/while nursing.

Appropriate engineering controls

Use local and general ventilation.

Individual protection measures (personal protective equipment)

Eye/face protection

Wear eye/face protection.

Hand protection

Protective gloves		
Material	Material thickness	Breakthrough times of the glove material
these information are not available	no information available	no information available

Unsuitable materials
Material
NR: natural rubber, latex
CR: chloroprene (chlorobutadiene) rubber
NBR: acrylonitrile-butadiene rubber
IIR: isobutene-isoprene (butyl) rubber
FKM: fluoro-elastomer
PVC: polyvinyl chloride

Wear suitable gloves.

Chemical protection gloves are suitable, which are tested according to EN 374.

Check leak-tightness/impermeability prior to use.

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.

Body protection

Protective clothing against liquid chemicals.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

Type: ABEK (combined filters against gases and vapors, color code: Brown/Grey/Yellow/Green).

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Environmental exposure controls

Use appropriate container to avoid environmental contamination.
Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	liquid
Color	colorless - transparent
Odor	aromatic
Odor threshold	not determined

Other safety parameters

pH (value)	not determined (Concentrate)
Melting point/freezing point	-36 °C
Boiling point or initial boiling point and boiling range	139 °C
Flash point	43 °C (Closed Cup)
Evaporation rate	not determined
Flammability (solid, gas)	not relevant (fluid)
Lower and upper explosion limit	not determined
Vapor pressure	10.47 hPa at 25 °C
Density and/or relative density	
Density	1.336 g/ml at 20 °C (OECD Guideline 109)
Relative density	1.353 (water = 1)
Relative vapour density	6.23 at 20 °C (air = 1)
Solubility(ies)	
Water solubility	33.8 mg/l at 20 °C not miscible in any proportion (OECD Guideline 105)
Partition coefficient	
n-octanol/water (log KOW)	3.7 (25 °C)

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Soil organic carbon/water (log KOC)	2.624 – 2.725 (ECHA)
Auto-ignition temperature	600 °C at 998 mbar (EU method A.15)
Decomposition temperature	this information is not available
Viscosity	
Kinematic viscosity	0.76 mm ² /s at 20 °C 0.58 mm ² /s at 40 °C (OECD Guideline 114)
Dynamic viscosity	1.01 mPa s at 20 °C 0.78 mPa s at 40 °C (OECD Guideline 114)
Explosive properties	none
Oxidizing properties	none
Information for relevant hazard classes according to GHS	
Flammable liquids	category 3: flammable liquid

9.2 Other information

Temperature class (USA, acc. to NEC 500)	T1 (maximum permissible surface temperature on the equipment: 450°C)
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SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

If heated:

Risk of ignition.

10.2 Chemical stability

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

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

Heat.

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Take precautionary measures against static discharge.

Protect from moisture.

Use explosion-proof electrical/ventilating/lighting/equipment.

Use only non-sparking tools.

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10.5 Incompatible materials

strong oxidizer, bases

10.6 Hazardous decomposition products

Hydrogen chloride (HCl).

Hydrogen fluoride (HF).

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

If not otherwise specified the classification is based on:

Animal studies; Evidence from any other toxicity tests; Expert judgment (weight of evidence determination).

Classification acc. to OSHA "Hazard Communication Standard" (29 CFR 1910.1200)

Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	5,546 mg/kg	rat, male	-	ECHA
inhalation: dust/mist	LC50	>32.03 mg/l/4h	rat	OECD Guideline 403	ECHA
inhalation: dust/mist	LC0	>32.03 mg/l/4h	rat	OECD Guideline 403	ECHA
dermal	LD50	>3,300 mg/kg	rabbit	-	ECHA
dermal	LD0	>3,300 mg/kg	rabbit	-	ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

(ECHA)

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

(ECHA)

Respiratory or skin sensitization

Skin sensitization

May cause an allergic skin reaction.

(ECHA, OECD Guideline 429)

Respiratory sensitization

Classification could not be established because:

Data are lacking, inconclusive, or conclusive but not sufficient for classification.

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Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.
(ECHA, OECD Guideline 471)

Carcinogenicity

Suspected of causing cancer (if inhaled).
(ECHA)

IARC Monographs

IARC Monographs on the Evaluation of Carcinogenic Risks to Humans			
Name of substance	CAS No	Classification	Number
4-chlorobenzotrifluoride	98-56-6	2B	-

Legend

2B Possibly carcinogenic to humans

National Toxicology Program (United States)

not listed

OSHA Carcinogens

Not listed.

Reproductive toxicity

Suspected of damaging the unborn child (if inhaled).
Suspected of damaging fertility (if inhaled).
(ECHA, OECD Guideline 415)

Specific target organ toxicity - single exposure

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

Specific target organ toxicity - repeated exposure

Exposure route	Endpoint	Value	Exposure time	Species	Method	Source
oral	LOEL	40 mg/kg bw /day	90 d	rat		ECHA
oral	NOAEL	40 mg/kg bw /day	90 d	rat		ECHA
oral	LOAEL	150 mg/kg bw /day	90 d	rat		ECHA

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

11.2 Other information

There is no additional information.

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SECTION 12: Ecological information

12.1 Toxicity

Aquatic toxicity (acute)

Based on available data, the classification criteria are not met.

Endpoint	Exposure time	Value	Species	Method	Source
LC50	48 h	3 mg/l	zebra fish (Danio rerio)	OECD Guideline 203	ECHA

Aquatic toxicity (chronic)

Based on available data, the classification criteria are not met.

Endpoint	Exposure time	Value	Species	Method	Source
EC50	30 min	242.1 mg/l	Activated sludge, municipal	OECD Guideline 209	ECHA
NOEC	72 h	0.41 mg/l	algae (pseudokirchneriella subcapitata)	OECD Guideline 201	ECHA
NOEC	3 h	3.2 mg/l	Activated sludge, municipal	OECD Guideline 209	ECHA
growth (EbCx) 10%	72 h	>0.41 mg/l	algae (pseudokirchneriella subcapitata)	OECD Guideline 201	ECHA
growth (EbCx) 20%	72 h	>0.41 mg/l	algae (pseudokirchneriella subcapitata)	OECD Guideline 201	ECHA
growth rate (ErCx) 10%	72 h	>0.41 mg/l	algae (pseudokirchneriella subcapitata)	OECD Guideline 201	ECHA
growth rate (ErCx) 20%	72 h	>0.41 mg/l	algae (pseudokirchneriella subcapitata)	OECD Guideline 201	ECHA

12.2 Persistence and degradability

Biodegradation

Not readily biodegradable.

Process of degradability				
Process	Degradation rate	Time	Method	Source
oxygen depletion	19.2 %	28 d	OECD Guideline 301 D	ECHA

Persistence

No data available.

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12.3 Bioaccumulative potential

n-octanol/water (log KOW)	3.7 (25 °C)
BCF	121.8 – 202

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	2.624 – 2.725
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12.5 Results of PBT and vPvB assessment

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

12.6 Other adverse effects

Data are not available.

Remarks

Wassergefährdungsklasse, WGK (water hazard class): 2 (Hazardous to water)
Do not empty into drains or surface water.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

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/packages

Completely emptied packages can be recycled.
Handle contaminated packages in the same way as the substance itself.

Remarks

Please consider the relevant national or regional provisions.

SECTION 14: Transport information

14.1 UN number

DOT	UN2234
IMDG-Code	UN2234
ICAO-TI	UN2234

14.2 UN proper shipping name

DOT	Chlorobenzotrifluorides
IMDG-Code	CHLOROBENZOTRIFLUORIDES
ICAO-TI	Chlorobenzotrifluorides

14.3 Transport hazard class(es)

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	DOT	3
	IMDG-Code	3
	ICAO-TI	3
14.4	Packing group	
	DOT	III
	IMDG-Code	III
	ICAO-TI	III
14.5	Environmental hazards	hazardous to the aquatic environment
14.6	Special precautions for user	-
14.7	Transport in bulk according to IMO instruments	-
14.8	<u>Information for each of the UN Model Regulations</u>	
	Transport of dangerous goods by road or rail (49 CFR US DOT) Additional information	
	Particulars in the shipper's declaration	UN2234, Chlorobenzotrifluorides, 3, III, environmentally hazardous
	Danger label(s)	3, fish and tree
		
	Environmental hazards	yes (hazardous to the aquatic environment)
	Special provisions (SP)	B1, IB3, T2, TP1
	ERG No	130
	International Maritime Dangerous Goods Code (IMDG) Additional information	
	Marine pollutant	yes (hazardous to the aquatic environment)
	Danger label(s)	3, fish and tree
		
	Special provisions (SP)	-
	Excepted quantities (EQ)	E1
	Limited quantities (LQ)	5 L
	EmS	F-E, S-D

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Stowage category	A
Segregation group	10 - Liquid halogenated hydrocarbons.
International Civil Aviation Organization (ICAO-IATA/DGR) Additional information	
Environmental hazards	yes (hazardous to the aquatic environment)
Danger label(s)	3
	
Excepted quantities (EQ)	E1
Limited quantities (LQ)	10 L

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

National regulations (United States)

Toxic Substance Control Act (TSCA) Substance is listed (ACTIVE)

Superfund Amendment and Reauthorization Act (SARA TITLE III)

The List of Extremely Hazardous Substances and Their Threshold Planning Quantities (EPCRA Section 302, 304)

Not listed

Specific Toxic Chemical Listings (EPCRA Section 313)

Not listed

Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)

List of Hazardous Substances and Reportable Quantities (CERCLA section 102a) (40 CFR 302.4)

Not listed

Clean Air Act

Not listed

Right to Know Hazardous Substance List

Toxic or Hazardous Substance List (MA-TURA)

Not listed

Hazardous Substances List (MN-ERTK)

Not listed

Hazardous Substance List (NJ-RTK)

Not listed

Hazardous Substance List (Chapter 323) (PA-RTK)

Not listed

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Hazardous Substance List (RI-RTK)

Not listed

California Environmental Protection Agency (Cal/EPA): Proposition 65 - Safe Drinking Water and Toxic Enforcement Act of 1987

Proposition 65 List of chemicals			
Name acc. to inventory	CAS No	Remarks	Type of the toxicity
p-chloro- α,α,α -trifluorotoluene (para-Chlorobenzotrifluoride, PCBTF)	98-56-6	-	cancer

Drug precursors, Chemicals designated within the Controlled Substances Act, 21 U.S.C. § 802, paragraphs 34 (list I) and 35 (list II)

Not listed

SECTION 16: Other information, including date of preparation or last revision

Date of preparation: 2023-11-15

Date of last revision: 2025-03-19.

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
49 CFR US DOT	49 CFR U.S. Department of Transportation
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
DOT	Department of Transportation (USA)
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
EmS	Emergency Schedule
ERG No	Emergency Response Guidebook - Number
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IARC	International Agency for Research on Cancer
IARC Mono-graphs	IARC Monographs on the Evaluation of Carcinogenic Risks to Humans
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

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Abbr.	Descriptions of used abbreviations
IMDG-Code	International Maritime Dangerous Goods Code
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
LOAEL	Lowest Observed Adverse Effect Level
LOEL	Lowest Observed Effect Level
NOAEL	No Observed Adverse Effect Level
NOEC	No Observed Effect Concentration
OSHA	Occupational Safety and Health Administration (United States)
PBT	Persistent, Bioaccumulative and Toxic
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

OSHA Hazard Communication Standard (HCS), 29 CFR 1910.1200.

Transport of dangerous goods by road or rail (49 CFR US DOT).

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 section 2 and 3)

Code	Text
H226	Flammable liquid and vapor.
H317	May cause an allergic skin reaction.
H351	Suspected of causing cancer (if inhaled).
H361	Suspected of damaging fertility or the unborn child (if inhaled).

Responsible for the safety data sheet

Chemical Regulatory Compliance Com- Telephone: +1 (630) 410-1660
pany e-Mail: GHS@crc-us.com
Jasper, GA Website: www.crc-us.com
USA

Disclaimer

This information is based upon the present state of our knowledge.

This SDS has been compiled and is solely intended for this product.