



# Chemical Analysis Report

Report 02-2022

Provided by:

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**Title:**

Chemical analysis of ethylene glycol

**Problem description:**

As ethylene glycol is proposed for hydrate prohibition, the hazardous effects as well as selected physical properties together with hazards categories are analyzed in this report.

**Summary:**

- Ethylene glycol has known health hazards, but not physical or environmental hazards.
- In health hazards, there is WARNING with respect to Oral toxicity (H302); Skin corrosion/irritation (H315); serious eye damage/irritation (H320); inhalation toxicity (H332).
- In health hazards, it is listed as DANGER with respect to reproductive toxicity (H360); specific target organ toxicity (H370, H372).
- Ethylene glycol is used as antifreeze in cooling and heating systems, in hydraulic brake fluids, as an industrial humectant, as an ingredient of electrolytic condensers, as a solvent in the paint and plastics industries, in the formulations of printers' inks, stamp pad inks, and inks for ballpoint pens, as a softening agent for cellophane, and in the synthesis of safety explosives, plasticizers, synthetic fibers and synthetic waxes.
- We would classify ethylene glycol as good, meaning it has a lot of applications because of favorable physical properties, but it must be used with caution and its release with water is a potential problem.

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## Physical properties

\*Blue text represents estimated value from PSEforSPEED in-house property estimation software

Primary properties		
Chemical	Unit	Ethylene Glycol
CAS no.		107-21-1
SMILE		OCCO
MW	g/mol	62.07
Tm	K	260.15
Tb	K	470.45
Tc	K	719.7
Pc	bar	76.99
Vc	cm <sup>3</sup> /mol	191
Zc	-	0.276
Gf[298K]	kJ/mol	-302.6
Hf[298K]	kJ/mol	-387.5
Omega	-	0.51
Hv[298K]	kJ/mol	62.46
Hv[Tb]	kJ/mol	49.07
Hfus	kJ/mol	9.95
Vm[298K]	cm <sup>3</sup> /mol	59.33
Sol.Par.[298K]	MPa <sup>1/2</sup>	33.7
SurfTens	dyn/cm	30.78
HansenD.sol	MPa <sup>1/2</sup>	17
HansenP.sol	MPa <sup>1/2</sup>	11
HansenH.sol	MPa <sup>1/2</sup>	26
Log(Kow)	-	-1.36
Log(Ws)	Log(mg/L)	6
pKa	-	15.1
AiT	K	685.928
Fp	K	384
Viscosity	cp	75.19
THERM.COND	mW/m-K	253
-Log(LC50)FM	Log(mol/L)	0.04
-Log(LC50)DM	Log(mol/L)	0.12

## Physical properties

Chemical	Unit	Ethylene Glycol
CAS no.		107-21-1
-Log(LD50)	Log(mol/kg)	1.12
Log(BCF)	-	0.15
-Log(PEL)	Log(mol/m <sup>3</sup> )	2.79
-Log(PCO)	-	0.07
Log(GWP)	-	N/A
Log(ODP)	-	N/A
Log(AP)	-	N/A
-LOG(EUAC)	Log(cas/kg)	4.99
-LOG(EUANonC)	Log(cas/kg)	6.4
-LOG(ERAC)	Log(cas/kg)	7.24
-LOG(ERANonC)	Log(cas/kg)	7.38
-LOG(EFWC)	Log(cas/kg)	4.27
-LOG(EFWNonC)	Log(cas/kg)	6.62
-LOG(ESWC)	Log(cas/kg)	9.33
-LOG(ESWNonC)	Log(cas/kg)	9.15
-LOG(ENSC)	Log(cas/kg)	6.55
-LOG(ENSNonC)	Log(cas/kg)	6.46
-LOG(EASC)	Log(cas/kg)	6.44
-LOG(EASNonC)	Log(cas/kg)	6.51
<b>Secondary properties</b>		
Zc	-	0.246
Sfus	J/(mol*K)	38.25
Vm[Tb]	cm <sup>3</sup> /mol	70.04
Refractive Index	-	1.4318
Molar Refraction	-	32.72
Closed Flash Temp.	K	385.16
Open Flash Temp.	K	383.69
Dipolar moment	debye	N/A
Dielectric const.	-	N/A
Henry[298K]	bar*m <sup>3</sup> /mol	6.08E+08
McGowan Volume	cm <sup>3</sup> /mol	50.78

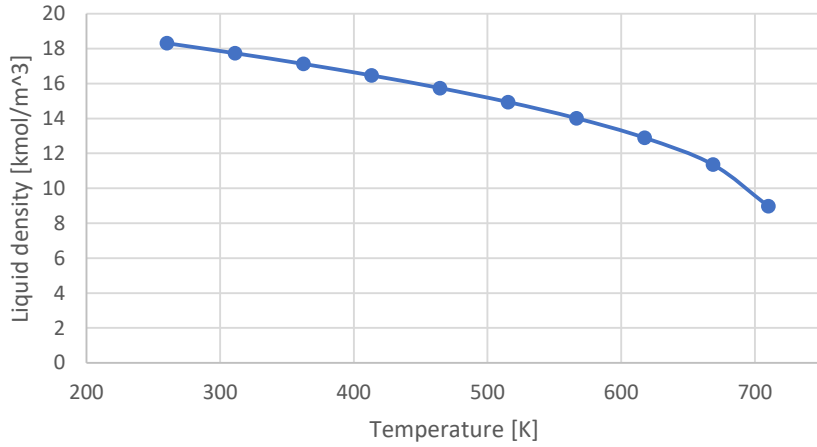
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Physical properties (T-dependent)

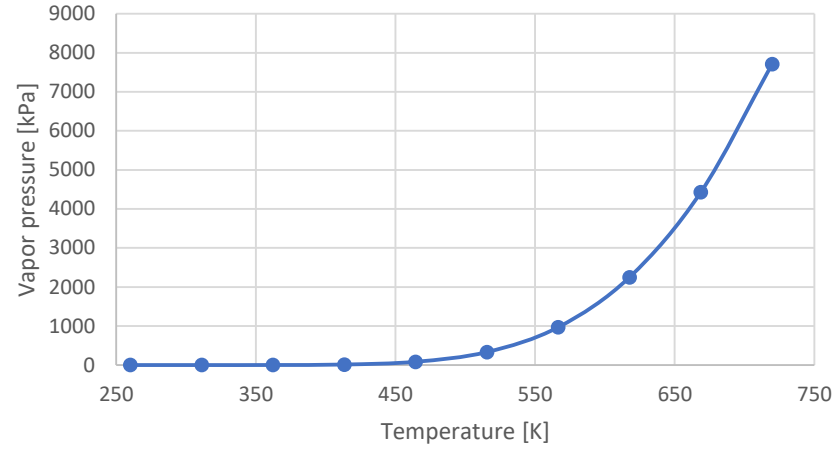
Please note that a sharp change of property in the plots indicate a phase change, which is not highlighted in the plots

Chemical Ethylene Glycol

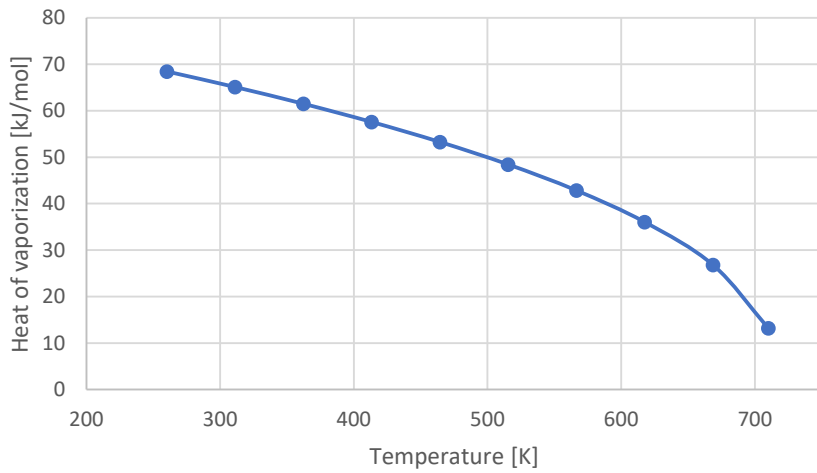
Liquid density vs T



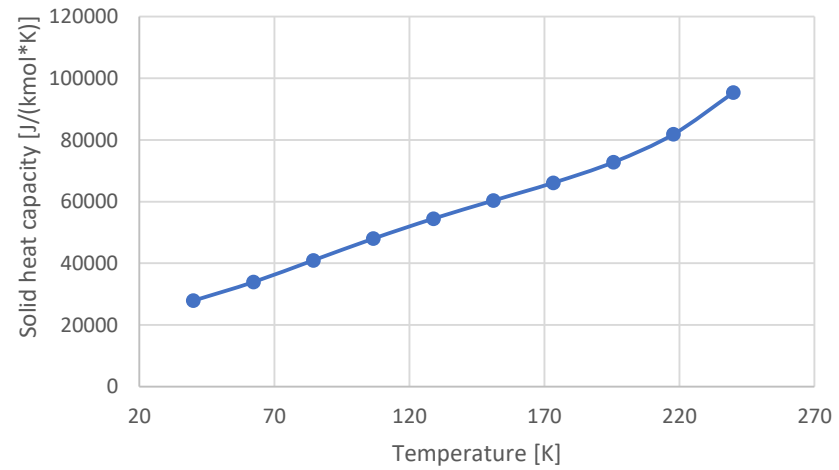
Vapor pressure vs T



Heat of vaporization vs T



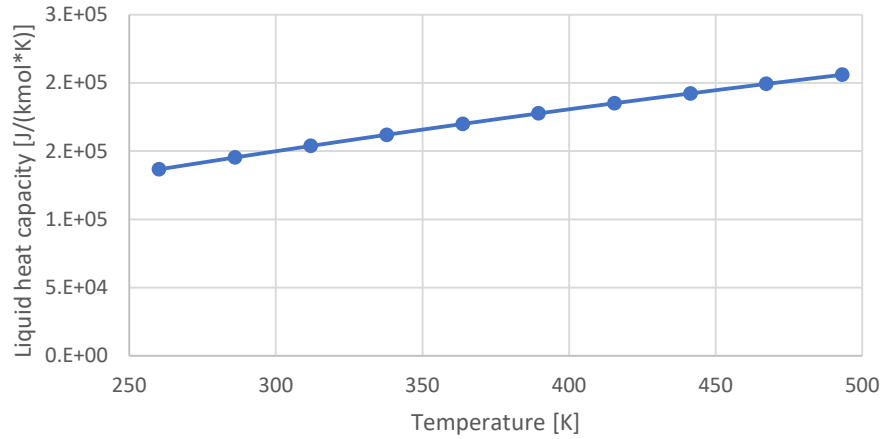
Solid heat capacity vs T



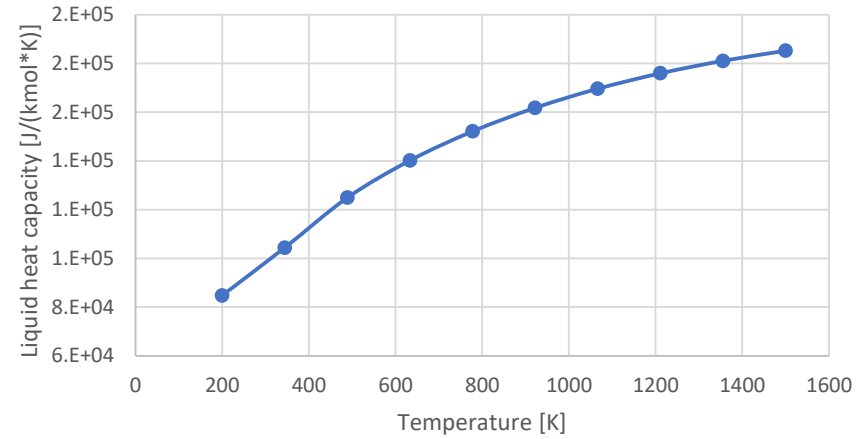
Please note that a sharp change of property in the plots indicate a phase change, which is not highlighted in the plots

Chemical Ethylene Glycol

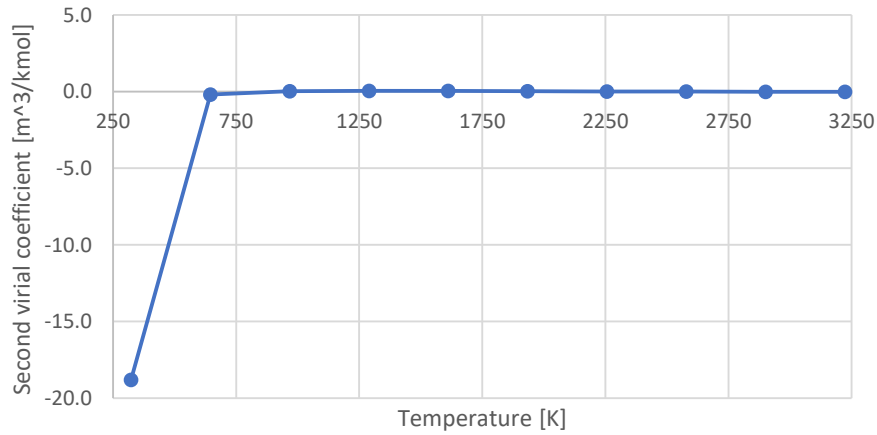
Liquid heat capacity vs T



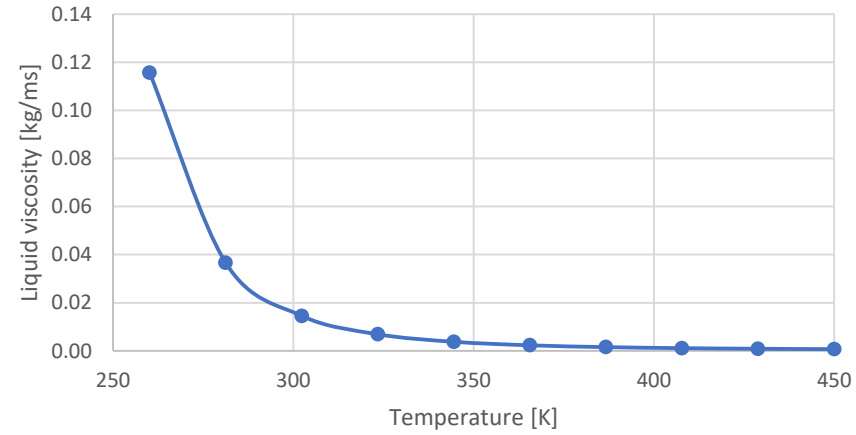
Ideal gas heat capacity vs T



Second virial coefficient vs T



Liquid viscosity vs T



Please note that a sharp change of property in the plots indicate a phase change, which is not highlighted in the plots

Chemical Ethylene Glycol

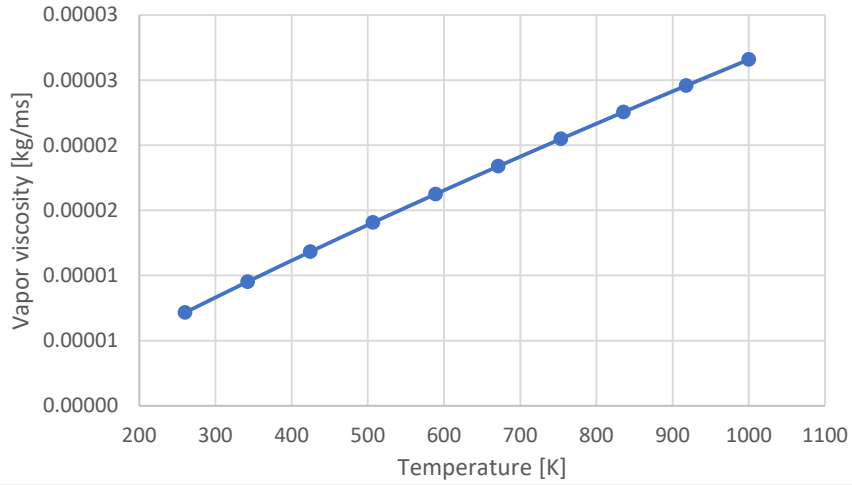
Vapor viscosity vs T

Liquid thermal conductivity vs T

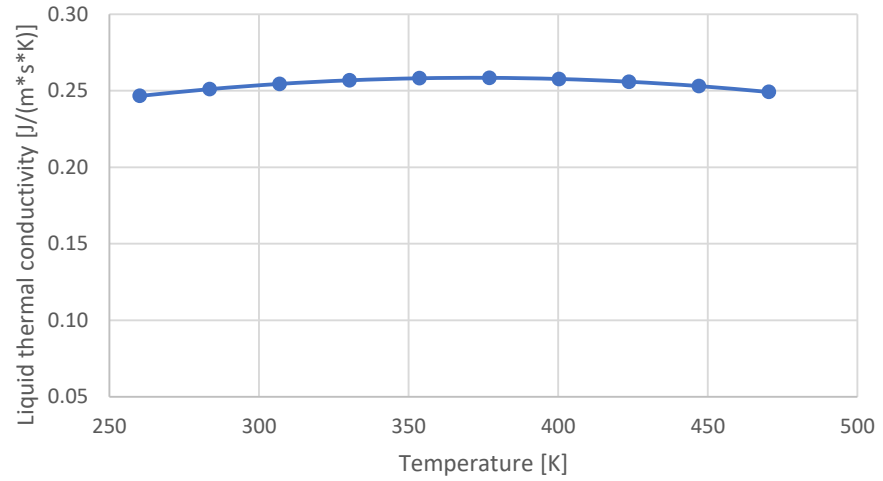
Physical properties (T-dependent)

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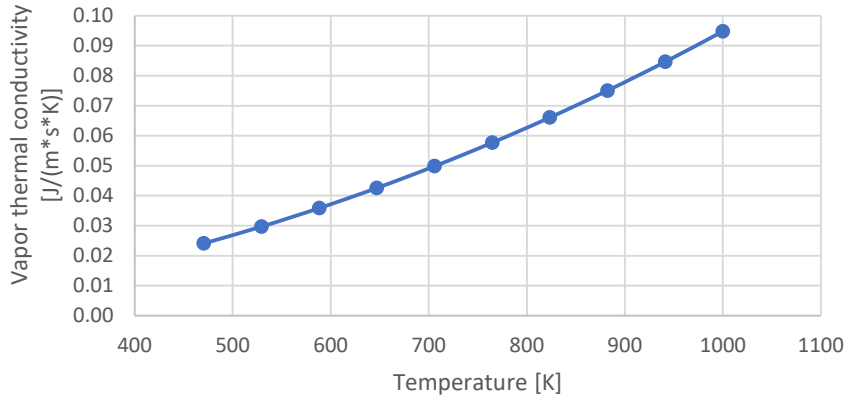
vapor viscosity vs T



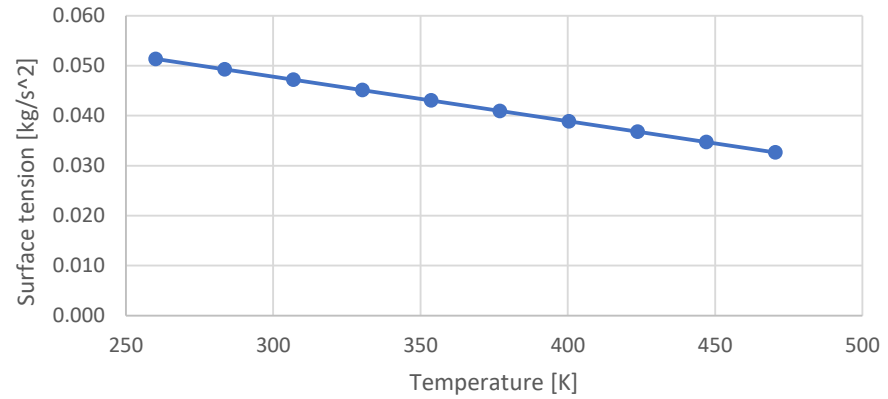
Liquid thermal conductivity vs T



Vapor thermal conductivity vs T



Surface tension vs T



Please note that a sharp change of property in the plots indicate a phase change, which is not highlighted in the plots

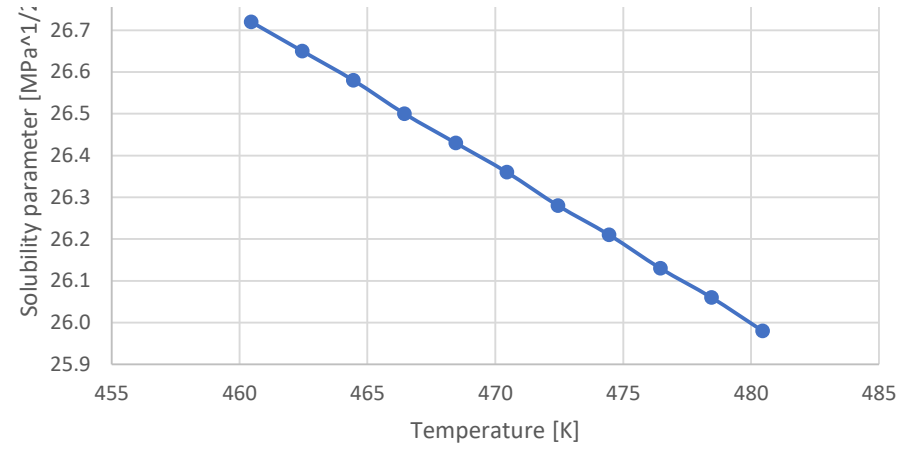
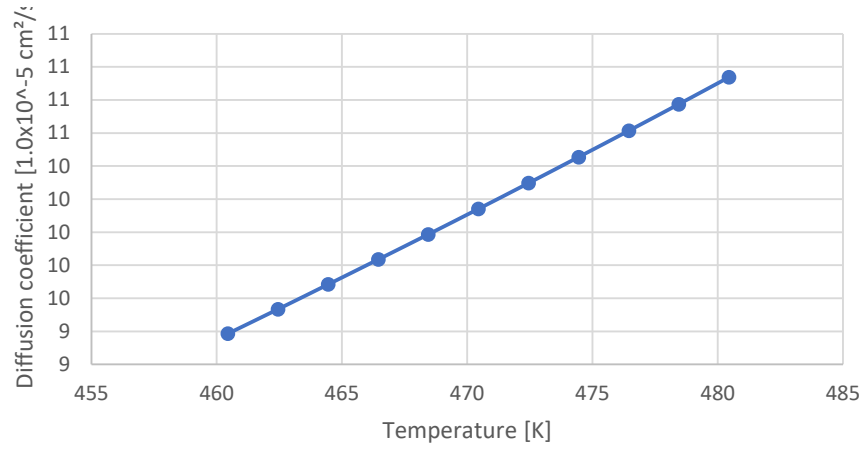
Chemical Ethylene Glycol

Diffusion coefficient at infinite dilution in water vs T (est.)

s]

Solubility parameter vs T (est.)

2] 26.8



Chemical	Ethylene Glycol
CAS no.	107-21-1
<b>Health hazard</b>	
Acute toxicity, oral	W(H302)
Skin corrosion/irritation	W(H315)
Serious eye damage/eye irritation	W(H320)
Acute toxicity, inhalation	W(H332)
Specific target organ toxicity, single exposure; Respiratory tract irritation	W(H335)
Reproductive toxicity	D(H360)
Specific target organ toxicity, single exposure	D(H370)
Specific target organ toxicity, repeated exposure	D(H372)

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**Physical hazard statement**

Code	Hazard Class (GHS Chapter)	Hazard Category	Signal Word
<b>Explosives</b>			
H200	Unstable Explosive	Unstable Explosive	Danger
H201	Explosive; mass explosion hazard	Div 1.1	Danger
H202	Explosive; severe projection hazard	Div 1.2	Danger
H203	Explosive; fire, blast or projection hazard	Div 1.3	Danger
H204	Fire or projection hazard	Div 1.4	Warning
H205	May mass explode in fire	Div 1.5	Danger
<b>Desensitized explosives</b>			
H206	Fire, blast or projection hazard; increased risk of explosion if desensitizing agent is reduced	Category 1	Danger
H207	Fire or projection hazard; increased risk of explosion if desensitizing agent is reduced	Category 2	Danger
H207	Fire or projection hazard; increased risk of explosion if desensitizing agent is reduced	Category 3	Warning
H208	Fire hazard; increased risk of explosion if desensitizing agent is reduced	Category 4	Warning
<b>Flammable gases</b>			
		1A: Flammable gas, Pyrophoric gas, Chemically unstable gas A,B	Danger
H220	Extremely flammable gas		Danger
H221	Flammable gas	1B	Danger
H221	Flammable gas	Category 2	Warning
<b>Flammable aerosol</b>			
H222	Extremely flammable aerosol	Category 1	Danger
H223	Flammable aerosol	Category 2	Warning
<b>Flammable liquids</b>			
H224	Extremely flammable liquid and vapor	Category 1	Danger
H225	Highly Flammable liquid and vapor	Category 2	Danger
H226	Flammable liquid and vapor	Category 3	Warning
H227	Combustible liquid	Category 4	Warning
<b>Flammable solids</b>			
H228	Flammable solid	Category 1	Danger
H228	Flammable solid	Category 2	Warning

## Hazard categories

<i>Aerosols</i>			
H229	Pressurized container: may burst if heated	Category 1	Danger
H229	Pressurized container: may burst if heated	Category 2	Warning
H229	Pressurized container: may burst if heated	Category 3	Warning
<i>Pyrophoric gas</i>			
H230	May react explosively even in the absence of air	1A, Chemically unstable gas A	
H231	May react explosively even in the absence of air at elevated pressure and/or temperature	1A, Chemically unstable gas B	
H232	May ignite spontaneously if exposed to air	1A, Pyrophoric gas	Danger
<i>Self-reactive substances and mixtures; Organic peroxides</i>			
H240	Heating may cause an explosion	Type A	Danger
H241	Heating may cause a fire or explosion	Type B	Danger
H242	Heating may cause a fire	Type C, D	Danger
H242	Heating may cause a fire	Type E, F	Warning
<i>Pyrophoric liquids, Pyrophoric solids</i>			
H250	Catches fire spontaneously if exposed to air	Category 1	Danger
<i>Self-heating substances and mixtures</i>			
H251	Self-heating; may catch fire	Category 1	Danger
H252	Self-heating in large quantities; may catch fire	Category 2	Warning
<i>Substances and mixtures which in contact with water, emit flammable gases</i>			
H260	In contact with water releases flammable gases which may ignite spontaneously	Category 1	Danger
H261	In contact with water releases flammable gas	Category 2	Danger
H261	In contact with water releases flammable gas	Category 3	Warning
<i>Oxidizing gases</i>			
H270	May cause or intensify fire; oxidizer	Category 1	Danger
<i>Oxidizing liquids, Oxidizing solids</i>			
H271	May cause fire or explosion; strong Oxidizer	Category 1	Danger
H272	May intensify fire; oxidizer	Category 2	Danger
H272	May intensify fire; oxidizer	Category 3	Warning
<i>Gases under pressure</i>			

H280	Contains gas under pressure; may explode if heated	Compressed gas, Liquefied gas, Dissolved gas	Warning
H281	Contains refrigerated gas; may cause cryogenic burns or injury	Refrigerated liquefied gas	Warning
	<b>Chemicals under pressure</b>		
H282	Extremely flammable chemical under pressure: may explode if heated	Category 1	Danger
H283	Flammable chemical under pressure: may explode if heated	Category 2	Warning
H284	Chemical under pressure: may explode if heated	Category 3	Warning
	<b>Corrosive to Metals</b>		
H290	May be corrosive to metals	Category 1	Warning

**Health hazard statement**

Code	Hazard Class (GHS Chapter)	Hazard Category	
	<b>Acute toxicity, oral</b>		
H300	Fatal if swallowed	Category 1, 2	Danger
H301	Toxic if swallowed	Category 3	Danger
H302	Harmful if swallowed	Category 4	Warning
H303	May be harmful if swallowed	Category 5	Warning
	<b>Aspiration hazard</b>		
H304	May be fatal if swallowed and enters airways	Category 1	Danger
H305	May be fatal if swallowed and enters airways	Category 2	Warning
	<b>Acute toxicity, dermal</b>		
H310	Fatal in contact with skin	Category 1, 2	Danger
H311	Toxic in contact with skin	Category 3	Danger
H312	Harmful in contact with skin	Category 4	Warning
H313	May be harmful in contact with skin	Category 5	
	<b>Skin corrosion/irritation</b>		
H314	Causes severe skin burns and eye damage	Category 1A, 1B, 1C	Danger
H315	Causes skin irritation	Category 2	Warning
H316	Causes mild skin irritation	Category 3	Warning

## Hazard categories

	<b>Sensitization, Skin</b>		
H317	May cause an allergic skin reaction	Category 1, 1A, 1B	Warning
	<b>Serious eye damage/eye irritation</b>		
H318	Causes serious eye damage	Category 1	Danger
H319	Causes serious eye irritation	Category 2A	Warning
H320	Causes eye irritation	Category 2B	Warning
	<b>Acute toxicity, inhalation</b>		
H330	Fatal if inhaled	Category 1, 2	Danger
H331	Toxic if inhaled	Category 3	Danger
H332	Harmful if inhaled	Category 4	Warning
H333	May be harmful if inhaled	Category 5	Warning
	<b>Sensitization, respiratory</b>		
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled	Category 1, 1A, 1B	Danger
	<b>Specific target organ toxicity, single exposure; Respiratory tract irritation</b>		
H335	May cause respiratory irritation	Category 3	Warning
H336	May cause drowsiness or dizziness	Category 3	Warning
	<b>Germ cell mutagenicity</b>		
H340	May cause genetic defects	Category 1A, 1B	Danger
H341	Suspected of causing genetic defects	Category 2	Warning
	<b>Carcinogenicity</b>		
H350	May cause cancer	Category 1A, 1B	Danger
H350i	May cause cancer by inhalation	Category 1A, 1B	Danger
H351	Suspected of causing cancer	Category 2	Warning
	<b>Reproductive toxicity</b>		
H360	May damage fertility or the unborn child	Category 1A, 1B	Danger
H360F	May damage fertility	Category 1A, 1B	Danger
H360D	May damage the unborn child	Category 1A, 1B	Danger
H360FD	May damage fertility; May damage the unborn child	Category 1A, 1B	Danger
H360Fd	May damage fertility; Suspected of damaging the unborn child	Category 1A, 1B	Danger
H360Df	May damage the unborn child; Suspected of damaging fertility	Category 1A, 1B	Danger
H361	Suspected of damaging fertility or the unborn child	Category 2	Warning
H361f	Suspected of damaging fertility	Category 2	Warning
H361d	Suspected of damaging the unborn child	Category 2	Warning

## Hazard categories

H361fd	Suspected of damaging fertility; Suspected of damaging the unborn child	Category 2	Warning
H362	May cause harm to breast-fed children	Additional category	
	<i>Specific target organ toxicity, single exposure</i>		
H370	Causes damage to organs	Category 1	Danger
H371	May cause damage to organs	Category 2	Warning
	<i>Specific target organ toxicity, repeated exposure</i>		
H372	Causes damage to organs through prolonged or repeated exposure	Category 1	Danger
H373	Causes damage to organs through prolonged or repeated exposure	Category 2	Warning

## Environmental hazard statement

Code	Hazard Class (GHS Chapter)	Hazard Category	
	<i>Hazardous to the aquatic environment, acute hazard</i>		
H400	Very toxic to aquatic life	Category 1	Warning
H401	Toxic to aquatic life	Category 2	
H402	Harmful to aquatic life	Category 3	
	<i>Hazardous to the aquatic environment, long-term hazard</i>		
H410	Very toxic to aquatic life with long lasting effects	Category 1	Warning
H411	Toxic to aquatic life with long lasting effects	Category 2	
H412	Harmful to aquatic life with long lasting effects	Category 3	
H413	May cause long lasting harmful effects to aquatic life	Category 4	
	<i>Hazardous to the ozone layer</i>		
H420	Harms public health and the environment by destroying ozone in the upper atmosphere	Category 1	Warning