

Thiophosgene

Other names:	Carbonothioic dichloride
	Carbon chlorosulfide
	Carbonic dichloride, thio-
	Dichlorothiocarbonyl
	Thiocarbonyl chloride
	Thiocarbonyl dichloride
	CSCI2
	Carbonyl chloride, thio-
	Phosgene, thio-
	Thiocarbonic dichloride
	Thiofosgen
	Thiokarbonylchlorid
	UN 2474
	Dichlorothioformaldehyde
Inchi:	InChI=1S/CCI2S/c2-1(3)4
InchiKey:	ZWZVWGITAAIFPS-UHFFFAOYSA-N
Formula:	CCI2S
SMILES:	S=C(Cl)Cl
Mol. weight [g/mol]:	114.98
CAS:	463-71-8

Physical Properties

Property code	Value	Unit	Source
affp	752.50	kJ/mol	NIST Webbook
basg	721.80	kJ/mol	NIST Webbook
gf	50.74	kJ/mol	Joback Method
hf	51.05	kJ/mol	Joback Method
hfl	21.10	kJ/mol	NIST Webbook
hfus	11.34	kJ/mol	Joback Method
hvap	33.32	kJ/mol	Joback Method
ie	9.68	eV	NIST Webbook
ie	9.61 ± 0.02	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.749		Crippen Method
mcvol	61.480	ml/mol	McGowan Method
pc	5953.74	kPa	Joback Method

tb	367.18	K	Joback Method
tc	587.44	K	Joback Method
tf	195.14	K	Joback Method
vc	0.226	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	68.94	J/mol×K	367.18	Joback Method
cpg	71.06	J/mol×K	403.89	Joback Method
cpg	72.82	J/mol×K	440.60	Joback Method
cpg	74.26	J/mol×K	477.31	Joback Method
cpg	75.43	J/mol×K	514.02	Joback Method
cpg	76.35	J/mol×K	550.73	Joback Method
cpg	77.07	J/mol×K	587.44	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C463718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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