CHLOROMETHYL THIOCYANATE

Other names: Thiocyanic acid chloromethyl ester
Chloromethylthiocyanogen
Inchi: InChI=1S/C2H2ClNS/c3-1-5-2-4/h1H2
InchiKey: UXUCVNXUWOLPRU-UHFFFAOYSA-N
Formula: C2H2ClNS
SMILES: N#CSCCl
Mol. weight [g/mol]: 107.56

Physical Properties

Property code	Value	Unit	Source
hfus	10.77	kJ/mol	Joback Method
ie	10.29	eV	NIST Webbook
logp	1.397		Crippen Method
mcvol	69.010	ml/mol	McGowan Method
tb	458.20	K	NIST Webbook
tf	240.47	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.24	J/mol×K	453.45	Joback Method
cpg	104.66	J/mol×K	491.79	Joback Method
cpg	107.92	J/mol×K	530.12	Joback Method
cpg	111.03	J/mol×K	568.46	Joback Method
cpg	113.98	J/mol×K	606.79	Joback Method
cpg	116.76	J/mol×K	645.13	Joback Method
cpg	119.37	J/mol×K	683.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	350.20	K	2.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3268799&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point