

Carbamothioic chloride, dimethyl-

Other names:	Carbamoyl chloride, dimethylthio- Dimethylthiocarbamoyl chloride Dimethylthiocarbamyl chloride N,N-Dimethylthiocarbamoyl chloride N,N-Dimethylthiocarbamyl chloride
Inchi:	InChI=1S/C3H6CINS/c1-5(2)3(4)6/h1-2H3
InchiKey:	PHWISQNXPLXQRU-UHFFFAOYSA-N
Formula:	C3H6CINS
SMILES:	CN(C)C(=S)Cl
Mol. weight [g/mol]:	123.60
CAS:	16420-13-6

Physical Properties

Property code	Value	Unit	Source
gf	190.29	kJ/mol	Joback Method
hf	93.04	kJ/mol	Joback Method
hfus	15.35	kJ/mol	Joback Method
hvap	35.43	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	1.072		Crippen Method
mcvol	87.400	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
tb	387.95	K	Joback Method
tc	593.05	K	Joback Method
tf	317.00 ± 4.00	K	NIST Webbook
tf	316.00 ± 3.00	K	NIST Webbook
tf	313.00 ± 5.00	K	NIST Webbook
tf	315.00 ± 4.00	K	NIST Webbook
tf	315.00 ± 3.00	K	NIST Webbook
tf	309.00 ± 3.00	K	NIST Webbook
tf	314.00 ± 4.00	K	NIST Webbook
tf	314.00 ± 4.00	K	NIST Webbook
tf	316.20 ± 2.00	K	NIST Webbook
tf	315.00 ± 4.00	K	NIST Webbook
tf	316.00 ± 3.00	K	NIST Webbook
tf	316.20 ± 2.00	K	NIST Webbook
tf	311.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.74	J/mol×K	387.95	Joback Method
cpg	144.34	J/mol×K	422.13	Joback Method
cpg	151.33	J/mol×K	456.32	Joback Method
cpg	157.77	J/mol×K	490.50	Joback Method
cpg	163.68	J/mol×K	524.69	Joback Method
cpg	169.11	J/mol×K	558.87	Joback Method
cpg	174.11	J/mol×K	593.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16420136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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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