

Hydrazinecarbodithioic acid, 1-methyl-, methyl ester

Other names:	Carbamic acid, 2-methyldithio-, methyl ester Methyl 2-methyldithiocarbamate 2-Methyldithiocarbamic acid, methyl ester
Inchi:	InChI=1S/C3H8N2S2/c1-5(4)3(6)7-2/h4H2,1-2H3
InchiKey:	QCEOBXKEQKMIAY-UHFFFAOYSA-N
Formula:	C3H8N2S2
SMILES:	CSC(=S)N(C)N
Mol. weight [g/mol]:	136.24
CAS:	20184-94-5

Physical Properties

Property code	Value	Unit	Source
gf	301.79	kJ/mol	Joback Method
hf	184.44	kJ/mol	Joback Method
hfus	20.48	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
ie	8.39	eV	NIST Webbook
log10ws	-1.30		Crippen Method
logp	0.440		Crippen Method
mcvol	101.490	ml/mol	McGowan Method
pc	5552.58	kPa	Joback Method
tb	491.83	K	Joback Method
tc	729.48	K	Joback Method
tf	307.97	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.66	J/molxK	491.83	Joback Method
cpg	205.31	J/molxK	531.44	Joback Method
cpg	213.24	J/molxK	571.05	Joback Method
cpg	220.54	J/molxK	610.65	Joback Method
cpg	227.23	J/molxK	650.26	Joback Method

cpg	233.40	J/mol×K	689.87	Joback Method
cpg	239.09	J/mol×K	729.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20184945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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