Dimethylcarbamothioic acid, O-isopropyl ester

Other names:	Dimethyl-O-(1-methylethyl) ester of carbamothioic acid
	Carbamothioic acid, dimethyl-, O-(1-methylethyl) ester
	Carbamic acid, dimethylthio-, O-isopropyl ester
	O-Isopropyl N,N-dimethylthiocarbamate
Inchi:	InChI=1S/C6H13NOS/c1-5(2)8-6(9)7(3)4/h5H,1-4H3
InchiKey:	NOFGKMSNOXEHOX-UHFFFAOYSA-N
Formula:	C6H13NOS
SMILES:	CC(C)OC(=S)N(C)C
Mol. weight [g/mol]:	147.24
CAS:	24060-02-4

Physical Properties

Property code	Value	Unit	Source
gf	120.04	kJ/mol	Joback Method
hf	-90.64	kJ/mol	Joback Method
hfus	16.59	kJ/mol	Joback Method
hvap	39.74	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.258		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	441.14	K	Joback Method
tc	636.91	K	Joback Method
tf	231.35	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.70	J/mol×K	441.14	Joback Method
cpg	256.66	J/mol×K	473.77	Joback Method
cpg	267.97	J/mol×K	506.40	Joback Method
cpg	278.66	J/mol×K	539.03	Joback Method
cpg	288.75	J/mol×K	571.66	Joback Method

cpg	298.29	J/mol×K	604.29	Joback Method
cpg	307.29	J/mol×K	636.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24060024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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