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

Physical Properties

Property code	Value	Unit	Source
hfus	16.59	kJ/mol	Joback Method
logp	1.258		Crippen Method
mcvol	123.300	ml/mol	McGowan 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24060024&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume