S-Isobutyl-N,N-dimethyldithiocarbamate

Inchi: InChI=1S/C7H15NS2/c1-6(2)5-10-7(9)8(3)4/h6H,5H2,1-4H3
InchiKey: AXYGKMMVBLDPMQ-UHFFFAOYSA-N
Formula: C7H15NS2
SMILES: CC(C)CSC(=S)N(C)C
Mol. weight [g/mol]: 177.33

Physical Properties

Property code	Value	Unit	Source
gf	266.58	kJ/mol	Joback Method
hf	62.81	kJ/mol	Joback Method
hfus	22.12	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.222		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	1485.00		NIST Webbook
tb	510.38	K	Joback Method
tc	726.74	K	Joback Method
tf	254.79	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.96	J/mol×K	510.38	Joback Method
cpg	326.57	J/mol×K	546.44	Joback Method
cpg	339.30	J/mol×K	582.50	Joback Method
cpg	351.21	J/mol×K	618.56	Joback Method
cpg	362.36	J/mol×K	654.62	Joback Method
cpg	372.79	J/mol×K	690.68	Joback Method
cpg	382.55	J/mol×K	726.74	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=R122220&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume