S-tert-Butyl-N,N-dimethyldithiocarbamate

Inchi: InChI=1S/C7H15NS2/c1-7(2,3)10-6(9)8(4)5/h1-5H3
InchiKey: NIJRHTPLWSHTJQ-UHFFFAOYSA-N
Formula: C7H15NS2
SMILES: CN(C)C(=S)SC(C)(C)C
Mol. weight [g/mol]: 177.33

Physical Properties

Property code	Value	Unit	Source
gf	271.86	kJ/mol	Joback Method
hf	59.34	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	45.47	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.365		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1416.00		NIST Webbook
tb	507.59	K	Joback Method
tc	733.23	K	Joback Method
tf	272.21	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.98	J/mol×K	507.59	Joback Method
cpg	330.32	J/mol×K	545.20	Joback Method
cpg	343.57	J/mol×K	582.80	Joback Method
cpg	355.81	J/mol×K	620.41	Joback Method
cpg	367.11	J/mol×K	658.02	Joback Method
cpg	377.58	J/mol×K	695.62	Joback Method
cpg	387.28	J/mol×K	733.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R122280&Units=SI

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