Diisopropyldithiocarbamic acid

Inchi: InChI=1S/C7H15NS2/c1-5(2)8(6(3)4)7(9)10/h5-6H,1-4H3,(H,9,10)
InchiKey: GWXMDJKGVWQLBZ-UHFFFAOYSA-N
Formula: C7H15NS2
SMILES: CC(C)N(C(=S)S)C(C)C
Mol. weight [g/mol]: 177.33
CAS: 25022-55-3

Physical Properties

Property code	Value	Unit	Source
gf	260.41	kJ/mol	Joback Method
hf	-17.90 ± 1.70	kJ/mol	NIST Webbook
hfus	18.51	kJ/mol	Joback Method
hvap	45.91	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.320		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	504.02	K	Joback Method
tc	725.71	K	Joback Method
tf	241.85	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.11	J/mol×K	504.02	Joback Method
cpg	325.09	J/mol×K	540.97	Joback Method
cpg	338.11	J/mol×K	577.92	Joback Method
cpg	350.23	J/mol×K	614.87	Joback Method
cpg	361.52	J/mol×K	651.82	Joback Method
cpg	372.06	J/mol×K	688.76	Joback Method
cpg	381.90	J/mol×K	725.71	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=C25022553&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