N,N'-Di-sec-butylthiourea

Inchi: InChI=1S/C9H20N2S/c1-5-7(3)10-9(12)11-8(4)6-2/h7-8H,5-6H2,1-4H3,(H2,10,11,12)
InchiKey: QTOGVESSTRJHKB-UHFFFAOYSA-N
Formula: C9H20N2S
SMILES: CCC(C)NC(=S)NC(C)CC
Mol. weight [g/mol]: 188.33
CAS: 35700-30-2

Physical Properties

Property code	Value	Unit	Source
gf	315.86	kJ/mol	Joback Method
hf	13.79	kJ/mol	Joback Method
hfus	26.82	kJ/mol	Joback Method
hvap	54.45	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.047		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
tb	574.82	K	Joback Method
tc	774.34	K	Joback Method
tf	300.78	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.40	J/mol×K	574.82	Joback Method
cpg	430.04	J/mol×K	608.07	Joback Method
cpg	443.85	J/mol×K	641.33	Joback Method
cpg	456.89	J/mol×K	674.58	Joback Method
cpg	469.19	J/mol×K	707.84	Joback Method
cpg	480.81	J/mol×K	741.09	Joback Method
cpg	491.79	J/mol×K	774.34	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=C35700302&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