P-diisopropyl diphenyl thiourea

Inchi: InChI=1S/C19H24N2S/c1-13(2)15-5-9-17(10-6-15)20-19(22)21-18-11-7-16(8-12-18)14(3
InchiKey: CISCVXHQTKKFNJ-UHFFFAOYSA-N
Formula: C19H24N2S
SMILES: CC(C)c1ccc(NC(=S)Nc2ccc(C(C)C)cc2)cc1
Mol. weight [g/mol]: 312.47
CAS: 116496-66-3

Physical Properties

Property code	Value	Unit	Source
gf	605.62	kJ/mol	Joback Method
hf	257.51	kJ/mol	Joback Method
hfus	40.02	kJ/mol	Joback Method
hvap	82.59	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.742		Crippen Method
mcvol	263.060	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
tb	866.94	K	Joback Method
tc	1109.33	K	Joback Method
tf	491.36	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.11	J/mol×K	866.94	Joback Method
cpg	793.84	J/mol×K	907.34	Joback Method
cpg	808.52	J/mol×K	947.74	Joback Method
cpg	822.29	J/mol×K	988.13	Joback Method
cpg	835.28	J/mol×K	1028.53	Joback Method
cpg	847.64	J/mol×K	1068.93	Joback Method
cpg	859.49	J/mol×K	1109.33	Joback Method

Sources

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=C116496663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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