2,6-Diisopropylphenyl isothiocyanate

Inchi: InChI=1S/C13H17NS/c1-9(2)11-6-5-7-12(10(3)4)13(11)14-8-15/h5-7,9-10H,1-4H3
InchiKey: HZGOUCYIYIFQHX-UHFFFAOYSA-N
Formula: C13H17NS
SMILES: CC(C)c1cccc(C(C)C)c1N=C=S
Mol. weight [g/mol]: 219.35
CAS: 25343-70-8

Physical Properties

Property code	Value	Unit	Source
hf	175.45	kJ/mol	Joback Method
hvap	57.80	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.668		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	678.55	K	Joback Method
tc	923.04	K	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=C25343708&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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