2,6-Diethylphenyl isothiocyanate

Inchi: InChI=1S/C11H13NS/c1-3-9-6-5-7-10(4-2)11(9)12-8-13/h5-7H,3-4H2,1-2H3
InchiKey: QDPPZHPTDMQNBE-UHFFFAOYSA-N
Formula: C11H13NS
SMILES: CCc1cccc(CC)c1N=C=S
Mol. weight [g/mol]: 191.29
CAS: 25343-69-5

Physical Properties

Property code	Value	Unit	Source
hf	227.29	kJ/mol	Joback Method
hvap	54.12	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.546		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
tb	633.67	K	Joback Method
tc	878.48	K	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=C25343695&Units=SI

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