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:	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
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

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