

# 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](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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

<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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