

# 4-Diethylaminophenyl isothiocyanate

<b>Inchi:</b>	InChI=1S/C11H14N2S/c1-3-13(4-2)11-7-5-10(6-8-11)12-9-14/h5-8H,3-4H2,1-2H3
<b>InchiKey:</b>	PGWXUTHWTCRUAM-UHFFFAOYSA-N
<b>Formula:</b>	C11H14N2S
<b>SMILES:</b>	CCN(CC)c1ccc(N=C=S)cc1
<b>Mol. weight [g/mol]:</b>	206.31
<b>CAS:</b>	84381-54-4

## Physical Properties

Property code	Value	Unit	Source
hf	306.29	kJ/mol	Joback Method
hvap	55.50	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.267		Crippen Method
mcvol	169.800	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	641.13	K	Joback Method
tc	880.81	K	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C84381544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C84381544&amp;Units=SI</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	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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