

# 4-Decylphenyl isothiocyanate

<b>Inchi:</b>	InChI=1S/C17H25NS/c1-2-3-4-5-6-7-8-9-10-16-11-13-17(14-12-16)18-15-19/h11-14H,2-
<b>InchiKey:</b>	KLRFMWXUZQXOFA-UHFFFAOYSA-N
<b>Formula:</b>	C17H25NS
<b>SMILES:</b>	CCCCCCCCCc1ccc(N=C=S)cc1
<b>Mol. weight [g/mol]:</b>	275.45
<b>CAS:</b>	206559-54-8

## Physical Properties

Property code	Value	Unit	Source
hf	114.92	kJ/mol	Joback Method
hvap	66.81	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.104		Crippen Method
mcvol	244.360	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
tb	765.97	K	Joback Method
tc	984.49	K	Joback Method

## Sources

<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=C206559548&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C206559548&amp;Units=SI</a>
<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>

## 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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