

# Decyl isothiocyanate

<b>Other names:</b>	Decane, 1-isothiocyanato-
<b>Inchi:</b>	InChI=1S/C11H21NS/c1-2-3-4-5-6-7-8-9-10-12-11-13/h2-10H2,1H3
<b>InchiKey:</b>	HFWWGJSMDPUEFD-UHFFFAOYSA-N
<b>Formula:</b>	C11H21NS
<b>SMILES:</b>	CCCCCCCCCN=C=S
<b>Mol. weight [g/mol]:</b>	199.36
<b>CAS:</b>	24540-94-1

## Physical Properties

Property code	Value	Unit	Source
hf	13.70	kJ/mol	Joback Method
hvap	50.52	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.230		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	1564.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	597.03	K	Joback Method
tc	795.95	K	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C24540941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C24540941&amp;Units=SI</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvac:</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>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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