

# Naphthalene, 1-isothiocyanato-

<b>Other names:</b>	1-Isothiocyantenaphthalene 1-Isothiocyantonaphthalene 1-Naftyliisothiokyanat 1-Naphthalene isothiocyanate 1-Naphthyl Isothiocyanate ANI ANIT Isothiocyanic acid, 1-naphthyl ester Kesscocide NSC 89741 Naphthalene, isothiocyanato- «alpha»-Naphthyl isothiocyanate «alpha»-Naphthysothiocyanate Â«alphaÂ»-Naphthyl isothiocyanate Â«alphaÂ»-Naphthysothiocyanate
<b>Inchi:</b>	InChI=1S/C11H7NS/c13-8-12-11-7-3-5-9-4-1-2-6-10(9)11/h1-7H
<b>InchiKey:</b>	JBDOSUUXMYMWQH-UHFFFAOYSA-N
<b>Formula:</b>	C11H7NS
<b>SMILES:</b>	S=C=Nc1cccc2cccc12
<b>Mol. weight [g/mol]:</b>	185.25
<b>CAS:</b>	551-06-4

## Physical Properties

Property code	Value	Unit	Source
hf	429.83	kJ/mol	Joback Method
hvap	55.10	kJ/mol	Joback Method
log10ws	-4.60		Aqueous Solubility Prediction Method
logp	3.574		Crippen Method
mcvol	140.360	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
tb	647.67	K	Joback Method
tc	925.63	K	Joback Method
tf	330.48	K	Aqueous Solubility Prediction Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C551064&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C551064&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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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
<b>tf:</b>	Normal melting (fusion) point

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