

# Naphthalene, 1-isocyanato-

<b>Other names:</b>	Isocyanic acid, 1-naphthyl ester «alpha»-Naphthyl isocyanate 1-Isocyanatonaphthalene 1-Naphthyl isocyanate
<b>Inchi:</b>	InChI=1S/C11H7NO/c13-8-12-11-7-3-5-9-4-1-2-6-10(9)11/h1-7H
<b>InchiKey:</b>	BDQNKCYCTYYMAA-UHFFFAOYSA-N
<b>Formula:</b>	C11H7NO
<b>SMILES:</b>	O=C=Nc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	169.18
<b>CAS:</b>	86-84-0

## Physical Properties

Property code	Value	Unit	Source
chs	-5355.50 ± 4.20	kJ/mol	NIST Webbook
hf	140.35	kJ/mol	Joback Method
hfs	26.00 ± 4.20	kJ/mol	NIST Webbook
hvap	54.19	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	2.807		Crippen Method
mcvol	129.880	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	568.39	K	Joback Method
tc	810.43	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=C86840&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C86840&amp;Units=SI</a>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase 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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