

# Octadecane, 1-isocyanato-

<b>Other names:</b>	Isocyanic acid, octadecyl ester n-Octadecyl isocyanate Baykanol OI Bykanol OI Mondur O Octadecyl isocyanate Stearyl isocyanate Tonco-70 1-Isocyanatooctadecane 1-Octadecyl isocyanate Millionate O NSC 66466
<b>Inchi:</b>	InChI=1S/C19H37NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-19-21/h2-18H2
<b>InchiKey:</b>	QWDQYHPOSSHSAW-UHFFFAOYSA-N
<b>Formula:</b>	C19H37NO
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCN=C=O
<b>Mol. weight [g/mol]:</b>	295.50
<b>CAS:</b>	112-96-9

## Physical Properties

Property code	Value	Unit	Source
chs	-12146.00 ± 4.20	kJ/mol	NIST Webbook
hf	-440.90	kJ/mol	Joback Method
hfs	-618.40 ± 4.20	kJ/mol	NIST Webbook
hvap	67.42	kJ/mol	Joback Method
log10ws	-11.27		Crippen Method
logp	6.584		Crippen Method
mcvol	285.820	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
tb	700.79	K	Joback Method
tc	869.63	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	77.80	kJ/mol	441.00	NIST Webbook

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## 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=C112969&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C112969&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>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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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