Octadecane, 1-isocyanato-

Other names:	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
Inchi:	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
InchiKey:	QWDQYHPOSSHSAW-UHFFFAOYSA-N
Formula:	C19H37NO
SMILES:	CCCCCCCCCCCCCCCCCCN=C=O
Mol. weight [g/mol]:	295.50
CAS:	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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112969&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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