

N-Nitroso-di-n-octylamine

Other names:	1-Octanamine, N-nitroso-N-(n-octyl)- Diocetylamine, N-nitroso- DiocetylNitrosamine DiocetylNitrosoamine N-DiocetylNitrosamine Nitrosodi-N-octylamine Diocytlamine, N-nitroso- Nitrosodiocetylamine Di-n-octyl nitrosamine 1-Octanamine, N-nitroso-N-octyl- NSC 38886
Inchi:	InChI=1S/C16H34N2O/c1-3-5-7-9-11-13-15-18(17-19)16-14-12-10-8-6-4-2/h3-16H2,1-2H
InchiKey:	FLYCLWANFMDRKT-UHFFFAOYSA-N
Formula:	C16H34N2O
SMILES:	CCCCCCCCCCN(CCCCCCCC)N=O
Mol. weight [g/mol]:	270.45
CAS:	6335-97-3

Physical Properties

Property code	Value	Unit	Source
hf	-474.23	kJ/mol	Joback Method
hvap	62.35	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.691		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	641.32	K	Joback Method
tc	802.54	K	Joback Method

Sources

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=C6335973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolt:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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