1-Octanamine, N-nitroso-N-octyl-

Other names:	1-Octanamine, N-nitroso-N-(n-octyl)-
	Dioctylamine, N-nitroso-
	Dioctylnitrosamine
	Dioctylnitrosoamine
	N-Dioctylnitrosamine
	Nitrosodi-N-octylamine
	Diocytlamine, N-nitroso-
	Nitrosodioctylamine
	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:	CCCCCCCCN(CCCCCCCC)N=O
Mol. weight [g/mol]:	270.46

Physical Properties

Property code	Value	Unit	Source
af	0.9406		Cheméo Relay (1.0)
gf	224.27	kJ/mol	Cheméo Relay (1.0, beta)
hf	-268.41	kJ/mol	Cheméo Relay (1.0)
hvap	82.82	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-5.64		Cheméo Relay (1.0)
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	590.95	K	Cheméo Relay (1.0)
tc	762.73	K	Cheméo Relay (1.0)
tf	312.04	K	Cheméo Relay (1.0)
vc	1.014	m3/kmol	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6335973&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/82-256-7/1-Octanamine-N-nitroso-N-octyl.pdf
Generated by Cheméo on 2026-07-21 03:51:20.422369026 +0000 UTC m=+116976.264254420.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.