

N,N-DIMETHYLOCTYLAMINE

Other names:	1-octanamine, N,N-dimethyl-Dimethyl-n-octylamine N,N-Dimethyl-n-octylamine N,N-dimethyl-1-octanamine N,N-dimethyloctanamine N-(n-Octyl)dimethylamine N-Octyldimethylamine Octylamine, N,N-dimethyl-dimethyloctylamine octyldimethylamine
Inchi:	InChI=1S/C10H23N/c1-4-5-6-7-8-9-10-11(2)3/h4-10H2,1-3H3
InchiKey:	UQKAOOAFEFCDGT-UHFFFAOYSA-N
Formula:	C10H23N
SMILES:	CCCCCCCCN(C)C
Mol. weight [g/mol]:	157.30
CAS:	7378-99-6

Physical Properties

Property code	Value	Unit	Source
af	0.5096		Cheméo Relay (1.0)
gf	144.10	kJ/mol	Joback Method
hf	-180.68	kJ/mol	Cheméo Relay (1.0)
hfus	24.68	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-3.04		Cheméo Relay (1.0)
logp	2.909		Crippen Method
mcvol	161.740	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
tb	464.15 ± 3.00	K	NIST Webbook
tb	467.15 ± 3.00	K	NIST Webbook
tb	462.65 ± 3.00	K	NIST Webbook
tb	468.20	K	NIST Webbook
tc	624.20	K	Cheméo Relay (1.0)
tf	219.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.20	J/mol×K	601.86	Joback Method
cpg	363.50	J/mol×K	467.51	Joback Method
cpg	378.81	J/mol×K	494.38	Joback Method
cpg	393.52	J/mol×K	521.25	Joback Method
cpg	407.65	J/mol×K	548.12	Joback Method
cpg	421.20	J/mol×K	574.99	Joback Method
cpg	347.57	J/mol×K	440.64	Joback Method
hvapt	54.00 ± 0.50	kJ/mol	303.50	NIST Webbook
hvapt	50.20	kJ/mol	444.00	NIST Webbook
pvap	29.84	kPa	420.20	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT
pvap	49.84	kPa	436.70	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT
pvap	69.83	kPa	448.20	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT

pvap	89.83	kPa	457.90	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52920e+01
Coeff. B	-4.24828e+03
Coeff. C	-7.01840e+01
Temperature range (K), min.	353.32
Temperature range (K), max.	495.84

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7378996&Units=SI
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.cheméo.com/doc/models/crippen_log10ws
Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT (1.0, beta):	https://www.doi.org/10.1021/je300568h
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure: Cheméo Relay (1.0):	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity

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

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