1-Hexadecanamine

Other names:	1-AMINOHEXADECANE
	1-Hexadecylamine
	Alamine 6
	Amine 16D
	Armeen 16D
	CETYLAMINE
	Cetylamin
	Hexadecylamine
	Hexyldecylamine
	Monohexadecylamine
	N-CETYLAMINE
	NSC 8489
	Nissan Amine PB
	Palmitamine
	Palmityl amine
	n-Hexadecylamine
Inchi:	InChI=1S/C16H35N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h2-17H2,1H3
InchiKey:	FJLUATLTXUNBOT-UHFFFAOYSA-N
Formula:	C16H35N
SMILES:	CCCCCCCCCCCCCCCCN
Mol. weight [g/mol]:	241.46
CAS:	143-27-1

Physical Properties

Property code	Value	Unit	Source
gf	150.29	kJ/mol	Joback Method
hf	-339.78	kJ/mol	Joback Method
hfus	42.39	kJ/mol	Joback Method
hvap	61.85	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.426		Crippen Method
mcvol	246.280	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
tb	603.00 ± 5.00	K	NIST Webbook
tb	603.20	K	NIST Webbook

tb	592.15	K	KDB
tb	595.70	K	NIST Webbook
tc	806.57	K	Joback Method
tf	319.95 ± 1.00	K	NIST Webbook
tf	319.92 ± 0.50	K	NIST Webbook
tf	320.15 ± 2.00	K	NIST Webbook
tf	318.15 ± 2.00	K	NIST Webbook
tf	319.00 ± 1.50	K	NIST Webbook
tf	319.15 ± 2.00	K	NIST Webbook
tf	319.00 ± 2.00	K	NIST Webbook
tf	318.75 ± 0.70	K	NIST Webbook
tf	319.40 ± 2.00	K	NIST Webbook
tf	318.00 ± 0.70	K	NIST Webbook
tf	316.00 ± 3.00	K	NIST Webbook
tf	320.20 ± 2.00	K	NIST Webbook
tf	318.15	K	KDB
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.65	J/mol×K	778.48	Joback Method
cpg	693.66	J/mol×K	638.01	Joback Method
cpg	712.41	J/mol×K	666.10	Joback Method
cpg	730.37	J/mol×K	694.20	Joback Method
cpg	747.54	J/mol×K	722.29	Joback Method
cpg	763.96	J/mol×K	750.38	Joback Method
cpg	794.64	J/mol×K	806.57	Joback Method
hvapt	66.90	kJ/mol	553.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55671e+01
Coeff. B	-5.41889e+03
Coeff. C	-1.08270e+02

Temperature range (K), min.	462.92
Temperature range (K), max.	636.65

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.97379e+02
Coeff. B	-1.84700e+04
Coeff. C	-2.58979e+01
Coeff. D	1.04834e-05
Temperature range (K), min.	404.15
Temperature range (K), max.	595.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1285

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1285.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C143271&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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

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