1-Tetradecanamine

Other names:	1-AMINOTETRADECANE
	1-Tetradecylamine
	1838-04-6
	2016-54-8
	ARMEEN 14
	Alamine 5D
	Armeen 14D
	Monotetradecylamine
	Myristamine
	Myristylamine
	N-Tetradecylamine
	NSC 66437
	Tetradecanamine
	Tetradecylamine
Inchi:	InChI=1S/C14H31N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h2-15H2,1H3
InchiKey:	PLZVEHJLHYMBBY-UHFFFAOYSA-N
Formula:	C14H31N
SMILES:	CCCCCCCCCCCCCCN
Mol. weight [g/mol]:	213.40
CAS:	2016-42-4

Physical Properties

Property code	Value	Unit	Source
gf	133.45	kJ/mol	Joback Method
hf	-298.50	kJ/mol	Joback Method
hfus	37.21	kJ/mol	Joback Method
hvap	57.40	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.646		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	1640.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1638.00		NIST Webbook
ripol	1925.00		NIST Webbook
ripol	1925.00		NIST Webbook

tb	564.40	K	NIST Webbook
tc	761.79	K	Joback Method
tf	310.00 ± 3.00	K	NIST Webbook
tf	310.00 ± 2.00	K	NIST Webbook
tf	311.05 ± 0.50	K	NIST Webbook
tf	311.26 ± 0.30	K	NIST Webbook
tf	311.34 ± 0.30	K	NIST Webbook
tf	310.00 ± 2.00	K	NIST Webbook
tf	310.75 ± 0.50	K	NIST Webbook
tf	311.20 ± 3.00	K	NIST Webbook
vc	0.849	m3/kmol	Joback Method
volm	2.66e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.82	J/mol×K	592.25	Joback Method
cpg	601.68	J/mol×K	620.51	Joback Method
cpg	618.78	J/mol×K	648.76	Joback Method
cpg	635.15	J/mol×K	677.02	Joback Method
cpg	650.82	J/mol×K	705.28	Joback Method
cpg	665.80	J/mol×K	733.53	Joback Method
cpg	680.11	J/mol×K	761.79	Joback Method
psub	1.20e-04	kPa	298.15	The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57230e+01
Coeff. B	-5.17846e+03
Coeff. C	-9.80670e+01
Temperature range (K), min.	433.56
Temperature range (K), max.	595.45

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.89098e+02
Coeff. B	-1.69120e+04
Coeff. C	-2.49854e+01
Coeff. D	1.18834e-05
Temperature range (K), min.	311.34
Temperature range (K), max.	722.30

Sources

The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je400498a
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1283
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.12.025
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2016424&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1283.mol

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
volm:	Molar Volume