1-Heptadecanamine

Other names:	1-Aminoheptadecane
	Heptadecylamine
	Margarylamine
	n-Heptadecylamine
Inchi:	InChI=1S/C17H37N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h2-18H2,1H3
InchiKey:	KAJZYANLDWUIES-UHFFFAOYSA-N
Formula:	C17H37N
SMILES:	CCCCCCCCCCCCCCCCCN
Mol. weight [g/mol]:	255.48
CAS:	4200-95-7

Physical Properties

Property code	Value	Unit	Source
gf	158.71	kJ/mol	Joback Method
hf	-360.42	kJ/mol	Joback Method
hfus	44.98	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.816		Crippen Method
mcvol	260.370	ml/mol	McGowan Method
pc	1281.91	kPa	Joback Method
rinpol	2233.00		NIST Webbook
rinpol	2233.00		NIST Webbook
tb	609.00	K	NIST Webbook
tb	609.20	K	NIST Webbook
tc	829.51	K	Joback Method
tf	273.15 ± 3.00	K	NIST Webbook
tf	322.15 ± 2.00	K	NIST Webbook
tf	321.15 ± 2.00	K	NIST Webbook
tf	322.15 ± 2.00	K	NIST Webbook
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.54	J/mol×K	660.89	Joback Method
cpg	769.71	J/mol×K	688.99	Joback Method
cpg	788.05	J/mol×K	717.10	Joback Method
cpg	805.58	J/mol×K	745.20	Joback Method
cpg	822.34	J/mol×K	773.30	Joback Method
cpg	838.34	J/mol×K	801.40	Joback Method
cpg	853.62	J/mol×K	829.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63089e+01
Coeff. B	-5.80740e+03
Coeff. C	-1.12440e+02
Temperature range (K), min.	474.92
Temperature range (K), max.	640.51

Sources

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=C4200957&Units=SI

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume