1-Hexadecanamine, N-methyl-

Other names: N-methylhexadecylamine
methylhexadecylamine
Inchi: InChI=1S/C17H37N/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-2/h18H,3-17H2,1-2H3
InchiKey: IHFXMTOFDQKABX-UHFFFAOYSA-N
Formula: C17H37N
SMILES: CCCCCCCCCCCCCCCCNC
Mol. weight [g/mol]: 255.48
CAS: 13417-08-8

Physical Properties

Property code	Value	Unit	Source
gf	181.65	kJ/mol	Joback Method
hf	-340.74	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	59.87	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.687		Crippen Method
mcvol	260.370	ml/mol	McGowan Method
pc	1242.46	kPa	Joback Method
rinpol	1888.00		NIST Webbook
tb	638.53	K	Joback Method
tc	801.33	K	Joback Method
tf	334.01	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.87	J/mol×K	638.53	Joback Method
cpg	753.24	J/mol×K	665.66	Joback Method
cpg	771.80	J/mol×K	692.80	Joback Method
cpg	789.58	J/mol×K	719.93	Joback Method
cpg	806.61	J/mol×K	747.06	Joback Method
cpg	822.90	J/mol×K	774.19	Joback Method

cpg	838.48	J/mol×K	801.33	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59162e+01
Coeff. B	-5.48558e+03
Coeff. C	-1.06324e+02
Temperature range (K), min.	457.32
Temperature range (K), max.	623.60

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13417088&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
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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