1-Hexanamine, N,N-dihexyl-

Other names: N,N-dihexyl-1-hexanamine
Tri-n-hexylamine
Trihexylamine
Inchi: InChI=1S/C18H39N/c1-4-7-10-13-16-19(17-14-11-8-5-2)18-15-12-9-6-3/h4-18H2,1-3H3
InchiKey: DIAIBWNEUYXDNL-UHFFFAOYSA-N
Formula: C18H39N
SMILES: CCCCCCN(CCCCCC)CCCCCC
Mol. weight [g/mol]: 269.51
CAS: 102-86-3

Physical Properties

Property code	Value	Unit	Source
chl	-12223.80 ± 1.50	kJ/mol	NIST Webbook
gf	211.46	kJ/mol	Joback Method
hf	-347.32	kJ/mol	Joback Method
hfl	-433.30 ± 1.50	kJ/mol	NIST Webbook
hfus	45.40	kJ/mol	Joback Method
hvap	57.70	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	6.029		Crippen Method
mcvol	274.460	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	536.70	K	NIST Webbook
tb	564.15 ± 2.00	K	NIST Webbook
tb	537.15 ± 3.00	K	NIST Webbook
tb	533.15 ± 4.00	K	NIST Webbook
tc	782.28	K	Joback Method
tf	325.09	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.55	J/mol×K	755.84	Joback Method
cpg	764.90	J/mol×K	623.68	Joback Method
cpg	785.25	J/mol×K	650.11	Joback Method
cpg	804.77	J/mol×K	676.55	Joback Method
cpg	823.47	J/mol×K	702.98	Joback Method
cpg	841.39	J/mol×K	729.41	Joback Method
cpg	874.99	J/mol×K	782.28	Joback Method
rhol	796.22	kg/m3	298.15	Partial molar volume of tertiary amines in methanol at T = 298.15 K. Solvation, shape and specific interactions

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57498e+01
Coeff. B	-4.96712e+03
Coeff. C	-9.04780e+01
Temperature range (K), min.	411.72
Temperature range (K), max.	566.33

Sources

Partial molar volume of tertiary amines in methanol at T = 298.15 K. Solvation, shape and specific interactions:	https://www.doi.org/10.1016/j.jct.2012.07.012
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=C102863&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume