1-Hexanamine, 2-ethyl-N-(2-ethylhexyl)-

Other names: 1-Hexylamine, 2-ethyl-N-(2-ethylhexyl)-
2,2'-Diethyldihexylamine
Bis(2-ethylhexyl)amine
Di(2-ethylhexyl)amine
Dihexylamine, 2,2'-diethyl-
NSC 5329

Inchi: InChI=1S/C16H35N/c1-5-9-11-15(7-3)13-17-14-16(8-4)12-10-6-2/h15-17H,5-14H2,1-4H3

InchiKey: SAIKULLUBZKPDA-UHFFFAOYSA-N

Formula: C16H35N

SMILES: CCCCC(CC)CNCC(CC)CCCC

Mol. weight [g/mol]: 241.46

CAS: 106-20-7

Physical Properties

Property code	Value	Unit	Source
gf	168.35	kJ/mol	Joback Method
hf	-330.66	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	56.87	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	5.009		Crippen Method
mcvol	246.280	ml/mol	McGowan Method
pc	1346.69	kPa	Joback Method
rinpol	1579.00		NIST Webbook
tb	614.77	K	Joback Method
tc	781.90	K	Joback Method
tf	292.74	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.80	J/mol×K	614.77	Joback Method
cpg	697.35	J/mol×K	642.63	Joback Method

cpg	716.07	J/mol×K	670.48	Joback Method
cpg	733.98	J/mol×K	698.34	Joback Method
cpg	751.10	J/mol×K	726.19	Joback Method
cpg	767.47	J/mol×K	754.05	Joback Method
cpg	783.09	J/mol×K	781.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40261e+01
Coeff. B	-4.53603e+03
Coeff. C	-9.52310e+01
Temperature range (K), min.	425.40
Temperature range (K), max.	615.74

Sources

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=C106207&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume