1-Hexanamine, N-hexyl-

Other names:	Bis(1-hexyl)amine
	Di-N-hexylamine
	Dihexylamine
	N,N-Dihexylamine
	N-Hexylhexanamine
	N-hexyl-1-hexanamine
	di-Normal-hexylamine
Inchi:	InChI=1S/C12H27N/c1-3-5-7-9-11-13-12-10-8-6-4-2/h13H,3-12H2,1-2H3
InchiKey:	PXSXRABJBXYMFT-UHFFFAOYSA-N
Formula:	C12H27N
SMILES:	CCCCCCNCCCCCC
Mol. weight [g/mol]:	185.35
CAS:	143-16-8

Physical Properties

Property code	Value	Unit	Source
gf	139.55	kJ/mol	Joback Method
hf	-237.54	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hvap	48.74	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.737		Crippen Method
mcvol	189.920	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	1345.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1505.00		NIST Webbook
tb	466.70	K	NIST Webbook
tb	466.65 ± 10.00	K	NIST Webbook
tc	688.55	K	Joback Method
tf	286.21 ± 0.30	K	NIST Webbook
tf	273.65 ± 1.00	K	NIST Webbook
tf	260.09 ± 0.15	K	NIST Webbook
tf	258.50 ± 0.60	K	NIST Webbook
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.99	J/mol×K	633.75	Joback Method
cpg	542.27	J/mol×K	661.15	Joback Method
cpg	464.54	J/mol×K	524.13	Joback Method
cpg	481.38	J/mol×K	551.53	Joback Method
cpg	497.56	J/mol×K	578.94	Joback Method
cpg	513.09	J/mol×K	606.34	Joback Method
cpg	555.97	J/mol×K	688.55	Joback Method
hvapt	70.80	kJ/mol	298.15	The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography
hvapt	55.10	kJ/mol	488.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.25966e+01
Coeff. B	-6.88479e+03
Coeff. C	-8.37500e+01
Temperature range (K), min.	392.36
Temperature range (K), max.	482.06

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C143168&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
The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2013.08.005
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume