1-Hexanamine, 2-ethyl-

Other names:	1-Amino-2-ethylhexan
	1-Amino-2-ethylhexane
	2-Ethyl-1-aminohexane
	2-Ethyl-1-hexanamine
	2-Ethyl-1-hexylamine
	2-Ethylhexanamine
	2-Ethylhexylamine
	Armeen L8D
	Hexylamine, 2-ethyl-
	UN 2276
	«beta»-Ethylhexylamine
	Â«betaÂ»-Ethylhexylamine
Inchi:	InChI=1S/C8H19N/c1-3-5-6-8(4-2)7-9/h8H,3-7,9H2,1-2H3
InchiKey:	LTHNHFOGQMKPOV-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCCCC(CC)CN
Mol. weight [g/mol]:	129.24
CAS:	104-75-6

Physical Properties

Property code	Value	Unit	Source
gf	80.49	kJ/mol	Joback Method
hf	-179.94	kJ/mol	Joback Method
hfus	18.15	kJ/mol	Joback Method
hvap	52.22	kJ/mol	NIST Webbook
log10ws	-1.71		Aqueous Solubility Prediction Method
logp	2.162		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	442.20	K	NIST Webbook
tc	635.72	K	Joback Method
tf	248.18	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.05	J/mol×K	605.52	Joback Method
cpg	292.68	J/mol×K	454.53	Joback Method
cpg	306.70	J/mol×K	484.73	Joback Method
cpg	320.12	J/mol×K	514.93	Joback Method
cpg	332.98	J/mol×K	545.13	Joback Method
cpg	345.29	J/mol×K	575.33	Joback Method
cpg	368.30	J/mol×K	635.72	Joback Method
hvapt	44.80	kJ/mol	394.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56878e+01
Coeff. B	-4.18511e+03
Coeff. C	-6.41230e+01
Temperature range (K), min.	335.88
Temperature range (K), max.	467.46

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104756&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume