

3-Hexanamine

Other names:	1-Ethylbutylamine 3-Aminohexane 3-Hexylamine Butylamine, 1-ethyl-
Inchi:	InChI=1S/C6H15N/c1-3-5-6(7)4-2/h6H,3-5,7H2,1-2H3
InchiKey:	HQLZFBUAULNEGP-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CCCC(N)CC
Mol. weight [g/mol]:	101.19
CAS:	16751-58-9

Physical Properties

Property code	Value	Unit	Source
gf	63.65	kJ/mol	Joback Method
hf	-138.66	kJ/mol	Joback Method
hfus	12.97	kJ/mol	Joback Method
hvap	39.20	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.524		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	388.65 ± 2.00	K	NIST Webbook
tc	592.91	K	Joback Method
tf	225.64	K	Joback Method
vc	0.395	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.01	J/mol×K	408.77	Joback Method
cpg	222.78	J/mol×K	439.46	Joback Method
cpg	234.07	J/mol×K	470.15	Joback Method
cpg	244.89	J/mol×K	500.84	Joback Method
cpg	255.25	J/mol×K	531.53	Joback Method

cpg	265.17	J/mol×K	562.22	Joback Method
cpg	274.66	J/mol×K	592.91	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.77611e+01
Coeff. B	-4.44225e+03
Coeff. C	-5.47880e+01
Temperature range (K), min.	309.02
Temperature range (K), max.	411.61

Sources

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/ci9903071
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=C16751589&Units=SI

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

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

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