

2-Hexanamine

Other names:	1-Methylpentylamine 2-Aminohehexane 2-Hexylamine Pentylamine, 1-methyl-
Inchi:	InChI=1S/C6H15N/c1-3-4-5-6(2)7/h6H,3-5,7H2,1-2H3
InchiKey:	WGBBUURBHXLGFM-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CCCCC(C)N
Mol. weight [g/mol]:	101.19
CAS:	5329-79-3

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
rinpol	720.00		NIST Webbook
tb	389.15 ± 3.00	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	1.56712e+01
Coeff. B	-3.26938e+03
Coeff. C	-9.33560e+01
Temperature range (K), min.	305.88
Temperature range (K), max.	408.94

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=C5329793&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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