Cyclopentanamine

Other names:	AMINO CYCLOPENTANE
	Cyclopentylamine
	aminocyclopentane
Inchi:	InChI=1S/C5H11N/c6-5-3-1-2-4-5/h5H,1-4,6H2
InchiKey:	NISGSNTVMOOSJQ-UHFFFAOYSA-N
Formula:	C5H11N
SMILES:	NC1CCCC1
Mol. weight [g/mol]:	85.15
CAS:	1003-03-8

Physical Properties

Property code	Value	Unit	Source
chl	-3444.50 ± 0.79	kJ/mol	NIST Webbook
gf	94.22	kJ/mol	Joback Method
hf	-54.86 ± 0.92	kJ/mol	NIST Webbook
hfl	-95.14 ± 0.84	kJ/mol	NIST Webbook
hfus	7.84	kJ/mol	Joback Method
hvap	40.20 ± 0.42	kJ/mol	NIST Webbook
hvap	40.20 ± 0.40	kJ/mol	NIST Webbook
hvap	40.30	kJ/mol	NIST Webbook
log10ws	-1.36		Crippen Method
logp	0.888		Crippen Method
mcvol	80.430	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
sl	241.04	J/mol×K	NIST Webbook
tb	381.20	K	NIST Webbook
tb	381.62 ± 0.20	K	NIST Webbook
tb	381.00 ± 6.00	K	NIST Webbook
tc	615.99	K	Joback Method
tf	187.45 ± 0.50	K	NIST Webbook
tf	187.45 ± 0.30	K	NIST Webbook
tt	190.45 ± 0.02	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.54	J/mol×K	437.34	Joback Method
cpg	222.65	J/mol×K	615.99	Joback Method
cpg	212.74	J/mol×K	580.26	Joback Method
cpg	202.21	J/mol×K	544.53	Joback Method
cpg	191.01	J/mol×K	508.80	Joback Method
cpg	179.13	J/mol×K	473.07	Joback Method
cpg	153.21	J/mol×K	401.61	Joback Method
cpl	181.21	J/mol×K	298.00	NIST Webbook
hfust	8.31	kJ/mol	190.40	NIST Webbook
hfust	0.48	kJ/mol	184.50	NIST Webbook
hfust	8.31	kJ/mol	190.40	NIST Webbook
hvapt	38.30	kJ/mol	368.00	NIST Webbook
sfust	43.65	J/mol×K	190.40	NIST Webbook
sfust	2.58	J/mol×K	184.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46343e+01
Coeff. B	-3.25532e+03
Coeff. C	-5.61860e+01
Temperature range (K), min.	283.09
Temperature range (K), max.	405.36

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1322.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15K:	https://www.doi.org/10.1016/j.jct.2011.04.017
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003038&Units=SI
Thermodynamic study of heptane + amine mixtures. V. Excess and solvation Gibbs energies:	https://www.doi.org/10.1016/j.fluid.2014.12.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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