Cyclopentanamine, 1-methyl-

Other names: 1-methylcyclopentanamine
Inchi: InChI=1S/C6H13N/c1-6(7)4-2-3-5-6/h2-5,7H2,1H3
InchiKey: TWASBYPJZBHZQJ-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CC1(N)CCCC1
Mol. weight [g/mol]: 99.17
CAS: 40571-45-7

Physical Properties

Property code	Value	Unit	Source
gf	97.15	kJ/mol	Joback Method
hf	-57.66	kJ/mol	Joback Method
hfus	4.13	kJ/mol	Joback Method
hvap	38.70	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.278		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	4374.18	kPa	Joback Method
rinpol	789.00		NIST Webbook
rinpol	789.00		NIST Webbook
tb	273.15 ± 4.00	K	NIST Webbook
tc	646.58	K	Joback Method
tf	275.44	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.21	J/mol×K	424.73	Joback Method
cpg	208.32	J/mol×K	461.71	Joback Method
cpg	222.22	J/mol×K	498.68	Joback Method
cpg	235.05	J/mol×K	535.66	Joback Method
cpg	246.92	J/mol×K	572.63	Joback Method
cpg	257.96	J/mol×K	609.61	Joback Method

cpg	268.29	J/mol×K	646.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37115e+01
Coeff. B	-3.25660e+03
Coeff. C	-5.07240e+01
Temperature range (K), min.	293.32
Temperature range (K), max.	438.41

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40571457&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

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

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
rinpol: Non-polar retention indices

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