Piperazine, 2-methyl-

Other names: 2-Methylpiperazine
Inchi: InChI=1S/C5H12N2/c1-5-4-6-2-3-7-5/h5-7H,2-4H2,1H3
InchiKey: JOMNTHCQHJPVAZ-UHFFFAOYSA-N
Formula: C5H12N2
SMILES: CC1CNCCN1
Mol. weight [g/mol]: 100.16
CAS: 109-07-9

Physical Properties

Property code	Value	Unit	Source
gf	191.09	kJ/mol	Joback Method
hf	-16.59	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	40.67	kJ/mol	Joback Method
log10ws	0.74		Aqueous Solubility Prediction Method
logp	-0.432		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
tb	430.45	K	Joback Method
tc	655.53	K	Joback Method
tf	363.55	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.54	J/mol×K	430.45	Joback Method
cpg	188.89	J/mol×K	467.96	Joback Method
cpg	202.62	J/mol×K	505.48	Joback Method
cpg	215.73	J/mol×K	542.99	Joback Method
cpg	228.22	J/mol×K	580.50	Joback Method
cpg	240.09	J/mol×K	618.02	Joback Method
cpg	251.33	J/mol×K	655.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.20	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53054e+01
Coeff. B	-3.93903e+03
Coeff. C	-5.96200e+01
Temperature range (K), min.	321.91
Temperature range (K), max.	453.76

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C109079&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume