2-Methylpyrrolidine

Other names: Pyrrolidine, 2-methyl-
Inchi: InChI=1S/C5H11N/c1-5-3-2-4-6-5/h5-6H,2-4H2,1H3
InchiKey: RGHPCLZJAFCTIK-UHFFFAOYSA-N
Formula: C5H11N
SMILES: CC1CCCN1
Mol. weight [g/mol]: 85.15
CAS: 765-38-8

Physical Properties

Property code	Value	Unit	Source
gf	115.48	kJ/mol	Joback Method
hf	-48.24	kJ/mol	Joback Method
hfus	12.23	kJ/mol	Joback Method
hvap	33.74	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.758		Crippen Method
mcvol	80.430	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	377.63	K	Joback Method
tc	584.50	K	Joback Method
tf	262.04	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.31	J/mol×K	377.63	Joback Method
cpg	151.20	J/mol×K	412.11	Joback Method
cpg	163.51	J/mol×K	446.59	Joback Method
cpg	175.25	J/mol×K	481.07	Joback Method
cpg	186.42	J/mol×K	515.54	Joback Method
cpg	197.05	J/mol×K	550.02	Joback Method
cpg	207.14	J/mol×K	584.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32514e+01
Coeff. B	-2.98284e+03
Coeff. C	-4.43300e+01
Temperature range (K), min.	274.42
Temperature range (K), max.	420.01

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765388&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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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