

Pyrrolidine, 3-methyl-

Other names:	3-Methylpyrrolidine
Inchi:	InChI=1S/C5H11N/c1-5-2-3-6-4-5/h5-6H,2-4H2,1H3
InchiKey:	KYINPWAJIVTFBW-UHFFFAOYSA-N
Formula:	C5H11N
SMILES:	CC1CCNC1
Mol. weight [g/mol]:	85.15
CAS:	34375-89-8

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	-0.76		Crippen Method
logp	0.616		Crippen Method
mcvol	80.430	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
sl	236.43	J/molxK	NIST Webbook
tb	377.63	K	Joback Method
tc	584.50	K	Joback Method
tf	170.40	K	NIST Webbook
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.26628e+01
Coeff. B	-2.79537e+03
Coeff. C	-4.23560e+01
Temperature range (K), min.	268.24
Temperature range (K), max.	422.61

Sources

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=C34375898&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
cpl:	Liquid phase 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

sl: Liquid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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