2,2-Dimethyl-pyrrolidine

Other names: Pyrrolidine, 2,2-dimethyl-
Inchi: InChI=1S/C6H13N/c1-6(2)4-3-5-7-6/h7H,3-5H2,1-2H3
InchiKey: PHODFIDDEBEGCS-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CC1(C)CCCN1
Mol. weight [g/mol]: 99.17
CAS: 35018-15-6

Physical Properties

Property code	Value	Unit	Source
gf	118.41	kJ/mol	Joback Method
hf	-53.64	kJ/mol	Joback Method
hfus	8.52	kJ/mol	Joback Method
hvap	34.81	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.148		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	746.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	746.00		NIST Webbook
tb	400.75	K	Joback Method
tc	615.52	K	Joback Method
tf	297.21	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.85	J/mol×K	400.75	Joback Method
cpg	191.91	J/mol×K	436.54	Joback Method
cpg	205.88	J/mol×K	472.34	Joback Method
cpg	218.87	J/mol×K	508.13	Joback Method
cpg	230.97	J/mol×K	543.93	Joback Method

cpg	242.28	J/mol×K	579.72	Joback Method
cpg	252.91	J/mol×K	615.52	Joback Method

Sources

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=C35018156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume