3,4-Dimethyl pyrrolidine (E)

Other names: Pyrrolidine, 3,4-dimethyl, trans
Inchi: InChI=1S/C6H13N/c1-5-3-7-4-6(5)2/h5-7H,3-4H2,1-2H3/t5-,6-/m1/s1
InchiKey: RDEHRKLSYJBKDV-PHDIDXHHSA-N
Formula: C6H13N
SMILES: CC1CNCC1C
Mol. weight [g/mol]: 99.17

Physical Properties

Property code	Value	Unit	Source
gf	116.19	kJ/mol	Joback Method
hf	-89.22	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	35.66	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	0.862		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	796.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	796.00		NIST Webbook
tb	395.84	K	Joback Method
tc	600.42	K	Joback Method
tf	269.07	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.49	J/mol×K	395.84	Joback Method
cpg	191.02	J/mol×K	429.94	Joback Method
cpg	204.93	J/mol×K	464.03	Joback Method
cpg	218.24	J/mol×K	498.13	Joback Method
cpg	230.95	J/mol×K	532.22	Joback Method
cpg	243.08	J/mol×K	566.32	Joback Method

cpg	254.63	J/mol×K	600.42	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=R405857&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