

2,2,4-Trimethyl-pyrrolidine

Inchi:	InChI=1S/C7H15N/c1-6-4-7(2,3)8-5-6/h6,8H,4-5H2,1-3H3
InchiKey:	AJMDMNYTTSGFEL-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CC1CNC(C)(C)C1
Mol. weight [g/mol]:	113.20
CAS:	35018-28-1

Physical Properties

Property code	Value	Unit	Source
gf	119.12	kJ/mol	Joback Method
hf	-94.62	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	36.73	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.394		Crippen Method
mvol	108.610	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	806.00		NIST Webbook
tb	418.96	K	Joback Method
tc	630.89	K	Joback Method
tf	304.24	K	Joback Method
vc	0.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.37	J/molxK	418.96	Joback Method
cpg	233.80	J/molxK	454.28	Joback Method
cpg	249.17	J/molxK	489.60	Joback Method
cpg	263.56	J/molxK	524.92	Joback Method
cpg	277.08	J/molxK	560.24	Joback Method
cpg	289.81	J/molxK	595.57	Joback Method
cpg	301.85	J/molxK	630.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35018281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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