

3,3,6,9,9-Pentamethyl-2,10-diazabicyclo(4.4.0)decane

Other names:	1,8-Naphthyridine, 1,2,3,4,4a,5,6,7-octahydro-2,2,4a,7,7-pentamethyl-2,2,4a,7,7-Pentamethyl-1,2,3,4,4a,5,6,7-octahydro[1,8]naphthyridine, 1,2,3,4,4a,5,6,7-octahydro-2,2,4a,7,7-pentamethyl-1,8-naphthyridine
Inchi:	InChI=1S/C13H24N2/c1-11(2)6-8-13(5)9-7-12(3,4)15-10(13)14-11/h6-9H2,1-5H3,(H,14,15)
InchiKey:	OEOPGVPCZRQSMQ-UHFFFAOYSA-N
Formula:	C13H24N2
SMILES:	CC1(C)CCC2(C)CCC(C)(C)NC2=N1
Mol. weight [g/mol]:	208.34
CAS:	69340-58-5

Physical Properties

Property code	Value	Unit	Source
affp	1039.30	kJ/mol	NIST Webbook
basg	1006.90	kJ/mol	NIST Webbook
gf	332.32	kJ/mol	Joback Method
hf	-10.22	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.126		Crippen Method
mcvol	187.970	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	629.84	K	Joback Method
tc	884.50	K	Joback Method
tf	515.38	K	Joback Method
vc	0.711	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.72	J/mol×K	629.84	Joback Method
cpg	560.87	J/mol×K	672.28	Joback Method
cpg	582.93	J/mol×K	714.73	Joback Method
cpg	604.36	J/mol×K	757.17	Joback Method

cpg	625.59	J/mol×K	799.61	Joback Method
cpg	647.08	J/mol×K	842.05	Joback Method
cpg	669.27	J/mol×K	884.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69340585&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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