5-methyl-1,2,3,4,5,6-hexahydro-7H-cyclopenta[b]p

Inchi: InChI=1S/C9H13NO/c1-6-5-8(11)9-7(6)3-2-4-10-9/h6,10H,2-5H2,1H3
InchiKey: VLZZXKFOOXABOV-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: CC1CC(=O)C2=C1CCCN2
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
gf	93.63	kJ/mol	Joback Method
hf	-146.68	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.233		Crippen Method
mcvol	123.200	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1438.00		NIST Webbook
rinpol	1438.00		NIST Webbook
tb	561.77	K	Joback Method
tc	806.04	K	Joback Method
tf	419.80	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.25	J/mol×K	561.77	Joback Method
cpg	320.02	J/mol×K	602.48	Joback Method
cpg	335.81	J/mol×K	643.19	Joback Method
cpg	350.63	J/mol×K	683.90	Joback Method
cpg	364.51	J/mol×K	724.62	Joback Method
cpg	377.45	J/mol×K	765.33	Joback Method
cpg	389.48	J/mol×K	806.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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