7-methyl-2,3,4,5,6,7-hexahydrocyclopent[b]azepin

Inchi: InChI=1S/C10H15NO/c1-7-6-8-4-2-3-5-11-9(8)10(7)12/h7,11H,2-6H2,1H3
InchiKey: RYGXXXQBRORLIJ-UHFFFAOYSA-N
Formula: C10H15NO
SMILES: CC1CC2=C(NCCCC2)C1=O
Mol. weight [g/mol]: 165.23

Physical Properties

Property code	Value	Unit	Source
gf	89.95	kJ/mol	Joback Method
hf	-173.48	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	51.30	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.623		Crippen Method
mcvol	137.290	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	1495.00		NIST Webbook
tb	588.92	K	Joback Method
tc	836.80	K	Joback Method
tf	427.55	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.36	J/mol×K	588.92	Joback Method
cpg	371.00	J/mol×K	630.23	Joback Method
cpg	388.49	J/mol×K	671.55	Joback Method
cpg	404.86	J/mol×K	712.86	Joback Method
cpg	420.10	J/mol×K	754.17	Joback Method
cpg	434.23	J/mol×K	795.49	Joback Method
cpg	447.26	J/mol×K	836.80	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U366032&Units=SI

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