2,3,4,5,6,7-hexahydro-cyclopent[b]azepin-8(1H)-o

Inchi: InChI=1S/C9H13NO/c11-8-5-4-7-3-1-2-6-10-9(7)8/h10H,1-6H2
InchiKey: XZTJVKYWRODILK-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: O=C1CCC2=C1NCCCC2
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
gf	89.24	kJ/mol	Joback Method
hf	-132.50	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.377		Crippen Method
mcvol	123.200	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	570.71	K	Joback Method
tc	824.07	K	Joback Method
tf	420.52	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.34	J/mol×K	570.71	Joback Method
cpg	319.68	J/mol×K	612.94	Joback Method
cpg	335.92	J/mol×K	655.16	Joback Method
cpg	351.09	J/mol×K	697.39	Joback Method
cpg	365.20	J/mol×K	739.62	Joback Method
cpg	378.26	J/mol×K	781.84	Joback Method
cpg	390.31	J/mol×K	824.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225126&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
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
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