6,7-dimethyl-2,3,6,7-tetrahydro-cyclopent[b]azepi

Inchi: InChI=1S/C11H15NO/c1-7-8(2)11(13)10-9(7)5-3-4-6-12-10/h3,5,7-8,12H,4,6H2,1-2H3
InchiKey: IWVJMIGICFUHHO-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CC1C(=O)C2=C(C=CCCN2)C1C
Mol. weight [g/mol]: 177.24

Physical Properties

Property code	Value	Unit	Source
gf	120.62	kJ/mol	Joback Method
hf	-156.68	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.645		Crippen Method
mcvol	147.080	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	606.29	K	Joback Method
tc	851.35	K	Joback Method
tf	435.34	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.08	J/mol×K	606.29	Joback Method
cpg	401.67	J/mol×K	647.13	Joback Method
cpg	419.11	J/mol×K	687.98	Joback Method
cpg	435.42	J/mol×K	728.82	Joback Method
cpg	450.58	J/mol×K	769.66	Joback Method
cpg	464.62	J/mol×K	810.50	Joback Method
cpg	477.53	J/mol×K	851.35	Joback Method

Sources

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=R225171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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