5-(1-hydroxyethylidene)-hexahydro-7H-cyclopenta

Inchi: InChI=1S/C10H13NO2/c1-6(12)8-5-9(13)10-7(8)3-2-4-11-10/h11-12H,2-5H2,1H3/b8-6+
InchiKey: BJPWZQDKNZJLFC-SOFGYWHQSA-N
Formula: C10H13NO2
SMILES: CC(O)=C1CC(=O)C2=C1CCCN2
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
gf	9.85	kJ/mol	Joback Method
hf	-232.97	kJ/mol	Joback Method
hfus	22.13	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.429		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
tb	688.02	K	Joback Method
tc	917.25	K	Joback Method
tf	492.53	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.11	J/mol×K	688.02	Joback Method
cpg	393.06	J/mol×K	726.23	Joback Method
cpg	405.21	J/mol×K	764.43	Joback Method
cpg	416.58	J/mol×K	802.64	Joback Method
cpg	427.20	J/mol×K	840.84	Joback Method
cpg	437.11	J/mol×K	879.05	Joback Method
cpg	446.33	J/mol×K	917.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225146&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