Cyclopentanecarboxylic acid, 3alpha-hydroxy-, gamma-lactone

Inchi: InChI=1S/C6H8O2/c7-6-4-1-2-5(3-4)8-6/h4-5H,1-3H2
InchiKey: PXIPIYIAXWNZCU-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: O=C1OC2CCC1C2
Mol. weight [g/mol]: 112.13
CAS: 5732-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-99.67	kJ/mol	Joback Method
hf	-297.43	kJ/mol	Joback Method
hfus	12.95	kJ/mol	Joback Method
hvap	37.70	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.712		Crippen Method
mcvol	81.120	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	449.20	K	Joback Method
tc	675.71	K	Joback Method
tf	284.53	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.83	J/mol×K	449.20	Joback Method
cpg	192.22	J/mol×K	486.95	Joback Method
cpg	204.80	J/mol×K	524.70	Joback Method
cpg	216.61	J/mol×K	562.45	Joback Method
cpg	227.68	J/mol×K	600.21	Joback Method
cpg	238.06	J/mol×K	637.96	Joback Method
cpg	247.76	J/mol×K	675.71	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=C5732978&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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