Cyclohexanecarboxylic acid, 1,3-dihydroxy-4,5-(isopropylidenedioxy)-, gamma-lactone, 1-acetate

Inchi: InChI=1S/C12H16O6/c1-6(13)16-12-4-7(15-10(12)14)9-8(5-12)17-11(2,3)18-9/h7-9H,4-5
InchiKey: HDESZAGGYOKPFH-UHFFFAOYSA-N
Formula: C12H16O6
SMILES: CC(=O)OC12CC(OC1=O)C1OC(C)(C)OC1C2
Mol. weight [g/mol]: 256.25
CAS: 14833-64-8

Physical Properties

Property code	Value	Unit	Source
gf	-433.06	kJ/mol	Joback Method
hf	-873.63	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	0.528		Crippen Method
mcvol	173.980	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	718.82	K	Joback Method
tc	961.19	K	Joback Method
tf	531.19	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.01	J/mol×K	718.82	Joback Method
cpg	569.44	J/mol×K	759.21	Joback Method
cpg	586.47	J/mol×K	799.61	Joback Method
cpg	603.36	J/mol×K	840.00	Joback Method
cpg	620.39	J/mol×K	880.40	Joback Method
cpg	637.85	J/mol×K	920.79	Joback Method
cpg	656.01	J/mol×K	961.19	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=C14833648&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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