1,2-Anhydro-3,4,5,6-alloinositol

Other names: α-Epoxyconduritol-e
Inchi: InChI=1S/C6H10O5/c7-1-2(8)4(10)6-5(11-6)3(1)9/h1-10H
InchiKey: ZHMWOVGZCINIHW-UHFFFAOYSA-N
Formula: C6H10O5
SMILES: [O]C1C([O])C([O])C2OC2C1[O]
Mol. weight [g/mol]: 162.14
CAS: 23559-36-6

Physical Properties

Property code	Value	Unit	Source
chs	-2884.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-906.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-17.44		Crippen Method
logp	-1.036		Crippen Method
mcvol	94.430	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23559366&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume