(-)-1,2:5,6-Di-O-cyclohexylidene-L-inositol, diacetate

Inchi: InChI=1S/C22H32O8/c1-13(23)25-15-16(26-14(2)24)18-20(30-22(28-18)11-7-4-8-12-22)19-17(15)27-21(29-19)9-5-3-6-10-21/h15-20H,3-12H2,1-2H3/t15-,16-,17+,18+,19-,20-/m0/s1

InchiKey: ZUFNLWFMJYRZHS-UHFFFAOYSA-N

Formula: C22H32O8

SMILES: CC(=O)OC1C(OC(C)=O)C2OC3(CCCCC3)OC2C2OC3(CCCCC3)OC12

Mol. weight [g/mol]: 424.48

Physical Properties

Property code	Value	Unit	Source
gf	-493.02	kJ/mol	Joback Method
hf	-1224.67	kJ/mol	Joback Method
hfus	56.82	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	2.752		Crippen Method
mcvol	304.900	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2664.50		NIST Webbook
rinpol	2664.50		NIST Webbook
tb	1013.20	K	Joback Method
tc	1264.20	K	Joback Method
tf	688.44	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1202.29	J/mol×K	1013.20	Joback Method
cpg	1231.45	J/mol×K	1055.03	Joback Method
cpg	1261.56	J/mol×K	1096.87	Joback Method
cpg	1293.02	J/mol×K	1138.70	Joback Method
cpg	1326.21	J/mol×K	1180.53	Joback Method
cpg	1361.53	J/mol×K	1222.37	Joback Method
cpg	1399.37	J/mol×K	1264.20	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=U380076&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume