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

Inchi: InChI=1S/C22H26F6O8/c23-21(24,25)17(29)31-11-12(32-18(30)22(26,27)28)14-16(36-2

InchiKey: NZBHEDMCLWMLFW-UHFFFAOYSA-N

Formula: C22H26F6O8

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

Mol. weight [g/mol]: 532.43

Physical Properties

Property code	Value	Unit	Source
gf	-1656.20	kJ/mol	Joback Method
hf	-2418.83	kJ/mol	Joback Method
hfus	60.47	kJ/mol	Joback Method
hvap	90.96	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	3.837		Crippen Method
mcvol	315.520	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	2199.70		NIST Webbook
rinpol	2199.70		NIST Webbook
tb	1002.36	K	Joback Method
tc	1235.03	K	Joback Method
tf	696.82	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.14	J/mol×K	1002.36	Joback Method
cpg	1265.99	J/mol×K	1041.14	Joback Method
cpg	1292.89	J/mol×K	1079.92	Joback Method
cpg	1321.22	J/mol×K	1118.69	Joback Method
cpg	1351.33	J/mol×K	1157.47	Joback Method
cpg	1383.61	J/mol×K	1196.25	Joback Method
cpg	1418.43	J/mol×K	1235.03	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=U380216&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume