myo-Inositol 3,4,5,6-tetraacetate, bis(trifluoroacetate) (isomer 1)

Inchi: InChI=1S/C18H18F6O12/c1-5(25)31-9-10(32-6(2)26)12(34-8(4)28)14(36-16(30)18(22,23
InchiKey: UZOWQPZKDVUDFC-UHFFFAOYSA-N
Formula: C18H18F6O12
SMILES: CC(=O)OC1C(OC(C)=O)C(OC(C)=O)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(C)=O
Mol. weight [g/mol]: 540.32

Physical Properties

Property code	Value	Unit	Source
gf	-2480.12	kJ/mol	Joback Method
hf	-3125.19	kJ/mol	Joback Method
hfus	59.94	kJ/mol	Joback Method
hvap	101.99	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	0.675		Crippen Method
mcvol	308.880	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	1627.60		NIST Webbook
tb	1054.34	K	Joback Method
tc	1295.77	K	Joback Method
tf	720.14	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.86	J/mol×K	1054.34	Joback Method
cpg	1071.08	J/mol×K	1094.58	Joback Method
cpg	1072.51	J/mol×K	1134.82	Joback Method
cpg	1071.09	J/mol×K	1175.05	Joback Method
cpg	1066.77	J/mol×K	1215.29	Joback Method
cpg	1059.50	J/mol×K	1255.53	Joback Method
cpg	1049.22	J/mol×K	1295.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380221&Units=SI
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

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