(-)-1,4-Ditosyl-2,3-O-isopropylidene-L-threitol

Other names:	(-)-1,4-di-O-Tosyl-2,3-O-isopropylidene-L-threitol L-O-Isopropylidene-2,3-dihydroxy-1,4-bis(p-tosyl)butane (4S,5S)-(-)-1,4-di-O-Tosyl-2,3-O-isopropylidene-L-threitol (-)-2,3-O-Isopropylidene-1,4-di-O-tosyl-L-threitol (-)-1,4-di-O-Tosyl-2,3-O-isopropylidene-threitol 1,3-Dioxolane-4,5-dimethanol, 2,2-dimethyl-, bis(4-methylbenzenesulfonate), (4S-trans)- (4S-trans)-2,2-dimethyl-1,3-dioxolane-4,5-dimethyl bis(toluene-p-sulphonate)
Inchi:	InChI=1S/C21H26O8S2/c1-15-5-9-17(10-6-15)30(22,23)26-13-19-20(29-21(3,4)28-19)14
InchiKey:	KPFDKWNWYAXRNJ-UHFFFAOYSA-N
Formula:	C21H26O8S2
SMILES:	Cc1ccc(S(=O)(=O)OCC2OC(C)(C)OC2COS(=O)(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	470.56
CAS:	37002-45-2

Physical Properties

Property code	Value	Unit	Source
gf	-972.18	kJ/mol	Joback Method
hf	-1426.75	kJ/mol	Joback Method
hfus	68.32	kJ/mol	Joback Method
hvap	117.81	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	2.934		Crippen Method
mcvol	328.030	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
tb	943.68	K	Joback Method
tc	1170.44	K	Joback Method
tf	605.35	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.17	J/mol×K	943.68	Joback Method
cpg	1070.50	J/mol×K	981.47	Joback Method

cpg	1085.61	J/mol×K	1019.27	Joback Method
cpg	1099.58	J/mol×K	1057.06	Joback Method
cpg	1112.51	J/mol×K	1094.86	Joback Method
cpg	1124.48	J/mol×K	1132.65	Joback Method
cpg	1135.58	J/mol×K	1170.44	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=C37002452&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