Trans-1,2-cyclopentanediol bis-p-toluene sulfonate

Inchi: InChI=1S/C19H22O6S2/c1-14-6-10-16(11-7-14)26(20,21)24-18-4-3-5-19(18)25-27(22,23

InchiKey: MIHIJVTXAJWZIP-UHFFFAOYSA-N

Formula: C19H22O6S2

SMILES: Cc1ccc(S(=O)(=O)OC2CCCC2OS(=O)(=O)c2ccc(C)cc2)cc1

Mol. weight [g/mol]: 410.50

CAS: 116401-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-803.58	kJ/mol	Joback Method
hf	-1116.37	kJ/mol	Joback Method
hfus	52.41	kJ/mol	Joback Method
hvap	105.80	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.335		Crippen Method
mcvol	288.110	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
tb	848.45	K	Joback Method
tc	1073.44	K	Joback Method
tf	510.01	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.06	J/mol×K	848.45	Joback Method
cpg	885.78	J/mol×K	885.95	Joback Method
cpg	899.59	J/mol×K	923.45	Joback Method
cpg	911.49	J/mol×K	960.95	Joback Method
cpg	921.47	J/mol×K	998.45	Joback Method
cpg	929.53	J/mol×K	1035.94	Joback Method
cpg	935.66	J/mol×K	1073.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401173&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume