2-Methyl-2-nitro-1,3-propanediol-di-p-toluenesulfo

Inchi: InChI=1S/C18H21NO8S2/c1-14-4-8-16(9-5-14)28(22,23)26-12-18(3,19(20)21)13-27-29(2
InchiKey: LMFKGBHKRFMVLT-UHFFFAOYSA-N
Formula: C18H21NO8S2
SMILES: Cc1ccc(S(=O)(=O)OCC(C)(COS(=O)(=O)c2ccc(C)cc2)[N+](=O)[O-])cc1
Mol. weight [g/mol]: 443.49
CAS: 18386-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-802.45	kJ/mol	Joback Method
hf	-1155.38	kJ/mol	Joback Method
hfus	58.76	kJ/mol	Joback Method
hvap	118.92	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	2.450		Crippen Method
mcvol	302.300	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	963.57	K	Joback Method
tc	1198.96	K	Joback Method
tf	638.11	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.13	J/mol×K	963.57	Joback Method
cpg	928.61	J/mol×K	1002.80	Joback Method
cpg	936.23	J/mol×K	1042.03	Joback Method
cpg	942.04	J/mol×K	1081.26	Joback Method
cpg	946.03	J/mol×K	1120.50	Joback Method
cpg	948.24	J/mol×K	1159.73	Joback Method
cpg	948.69	J/mol×K	1198.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18386500&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

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