2-Methyl-2-p-toluenesulfonylamino-1,3-propanedi di-p-toluenesulfonate

Inchi: InChI=1S/C25H29NO8S3/c1-19-5-11-22(12-6-19)35(27,28)26-25(4,17-33-36(29,30)23-1

Inchikey: KFKHTTSOQOFXGU-UHFFFAOYSA-N

Formula: C25H29NO8S3

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

Mol. weight [g/mol]: 567.70

CAS: 10405-52-4

Physical Properties

Property code	Value	Unit	Source
gf	-1055.43	kJ/mol	Joback Method
hf	-1463.92	kJ/mol	Joback Method
hfus	75.66	kJ/mol	Joback Method
hvap	145.92	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	3.460		Crippen Method
mcvol	397.820	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
tb	1101.50	K	Joback Method
tc	1348.82	K	Joback Method
tf	703.55	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.90	J/mol×K	1101.50	Joback Method
cpg	1252.90	J/mol×K	1142.72	Joback Method
cpg	1254.24	J/mol×K	1183.94	Joback Method
cpg	1252.94	J/mol×K	1225.16	Joback Method
cpg	1249.02	J/mol×K	1266.38	Joback Method
cpg	1242.53	J/mol×K	1307.60	Joback Method
cpg	1233.49	J/mol×K	1348.82	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=C10405524&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