ETHYLENE GLYCOL DI-P-TOSYLATE

Other names:	1,2-Ethanediol, 1,2-bis(4-methylbenzenesulfonate)
	1,2-Ethanediol, bis(4-methylbenzenesulfonate)
	Ethylene glycol di-p-tosylate
	ethylene di-p-toluenesulfonate
Inchi:	InChI=1S/C16H18O6S2/c1-13-3-7-15(8-4-13)23(17,18)21-11-12-22-24(19,20)16-9-5-14(
InchiKey:	LZIPBJBQQPZLOR-UHFFFAOYSA-N
Formula:	C16H18O6S2
SMILES:	Cc1ccc(S(=O)(=O)OCCOS(=O)(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	370.45

Physical Properties

Property code	Value	Unit	Source
hf	-823.30	kJ/mol	Cheméo Relay (1.0)
hfus	49.63	kJ/mol	Joback Method
hvap	129.15	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-4.07		Cheméo Relay (1.0)
logp	2.414		Crippen Method
mcvol	256.700	ml/mol	McGowan Method
tb	704.63	K	Cheméo Relay (1.0)
tf	366.37	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.46	J/mol×K	769.20	Joback Method
cpg	720.26	J/mol×K	804.37	Joback Method
cpg	733.69	J/mol×K	839.54	Joback Method
cpg	745.73	J/mol×K	874.71	Joback Method
cpg	756.37	J/mol×K	909.87	Joback Method
cpg	765.58	J/mol×K	945.04	Joback Method
cpg	773.37	J/mol×K	980.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6315522&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point