4-Ethyl-4-(p-toluenesulfonoxymethyl)-2-methyl-de

Other names: 4-Ethyl-4-(p-toluenesulfonoxymethyl)-2-methyl-delta
Inchi: InChI=1S/C14H19NO4S/c1-4-14(9-18-12(3)15-14)10-19-20(16,17)13-7-5-11(2)6-8-13/h5
InchiKey: MIMPOGKFEUESDC-UHFFFAOYSA-N
Formula: C14H19NO4S
SMILES: CCC1(COS(=O)(=O)c2ccc(C)cc2)COC(C)=N1
Mol. weight [g/mol]: 297.37
CAS: 116595-29-0

Physical Properties

Property code	Value	Unit	Source
gf	-321.71	kJ/mol	Joback Method
hf	-631.80	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	81.52	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.298		Crippen Method
mcvol	219.010	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	721.89	K	Joback Method
tc	949.00	K	Joback Method
tf	493.46	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.73	J/mol×K	721.89	Joback Method
cpg	646.44	J/mol×K	759.74	Joback Method
cpg	663.10	J/mol×K	797.59	Joback Method
cpg	678.80	J/mol×K	835.45	Joback Method
cpg	693.64	J/mol×K	873.30	Joback Method
cpg	707.70	J/mol×K	911.15	Joback Method
cpg	721.09	J/mol×K	949.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595290&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