3Beta-acetoxy-17beta-toluenesulfonoxy-5-andros

Inchi: InChI=1S/C28H38O5S/c1-18-5-8-22(9-6-18)34(30,31)33-26-12-11-24-23-10-7-20-17-21(
InchiKey: VHSUWQHYYVDVEW-UHFFFAOYSA-N
Formula: C28H38O5S
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(OS(=O)(=O)c4ccc(C)cc4)CCC32)C1
Mol. weight [g/mol]: 486.66
CAS: 1259-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-351.08	kJ/mol	Joback Method
hf	-950.39	kJ/mol	Joback Method
hfus	50.77	kJ/mol	Joback Method
hvap	109.30	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	5.963		Crippen Method
mcvol	375.280	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
tb	1057.11	K	Joback Method
tc	1304.60	K	Joback Method
tf	679.73	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1407.93	J/mol×K	1057.11	Joback Method
cpg	1439.04	J/mol×K	1098.36	Joback Method
cpg	1471.07	J/mol×K	1139.61	Joback Method
cpg	1504.40	J/mol×K	1180.86	Joback Method
cpg	1539.39	J/mol×K	1222.10	Joback Method
cpg	1576.42	J/mol×K	1263.35	Joback Method
cpg	1615.85	J/mol×K	1304.60	Joback Method

Sources

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=C1259229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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