anisomycin

Inchi: InChI=1S/C14H19NO4/c1-9(16)19-14-12(15-8-13(14)17)7-10-3-5-11(18-2)6-4-10/h3-6,12
InchiKey: YKJYKKNCCRKFSL-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: COc1ccc(CC2NCC(O)C2OC(C)=O)cc1
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
gf	-197.12	kJ/mol	Joback Method
hf	-578.87	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Joback Method
log10ws	-1.61		Aqueous Solubility Prediction Method
logp	0.502		Crippen Method
mcvol	202.660	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	796.76	K	Joback Method
tc	1010.67	K	Joback Method
tf	413.65	K	Aqueous Solubility Prediction Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.58	J/mol×K	796.76	Joback Method
cpg	640.04	J/mol×K	832.41	Joback Method
cpg	653.35	J/mol×K	868.06	Joback Method
cpg	665.51	J/mol×K	903.72	Joback Method
cpg	676.51	J/mol×K	939.37	Joback Method
cpg	686.35	J/mol×K	975.02	Joback Method
cpg	695.04	J/mol×K	1010.67	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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