Flumethasone

Other names: 6,9-difluoro-11,17-dihydroxy-17-(2-hydroxyacetyl)-10,13,16-trimethyl-6,7,8,11,12,14,15,1
Inchi: InChI=1S/C22H28F2O5/c1-11-6-13-14-8-16(23)15-7-12(26)4-5-19(15,2)21(14,24)17(27)
InchiKey: WXURHACBFYSXBI-UHFFFAOYSA-N
Formula: C22H28F2O5
SMILES: CC1CC2C3CC(F)C4=CC(=O)C=CC4(C)C3(F)C(O)CC2(C)C1(O)C(=O)CO
Mol. weight [g/mol]: 410.46

Physical Properties

Property code	Value	Unit	Source
gf	-744.95	kJ/mol	Joback Method
hf	-1272.85	kJ/mol	Joback Method
hfus	36.53	kJ/mol	Joback Method
hvap	119.57	kJ/mol	Joback Method
log10ws	-5.61		Aqueous Solubility Prediction Method
log10ws	-5.61		Estimated Solubility Method
logp	1.844		Crippen Method
mcvol	293.090	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
tb	1128.75	K	Joback Method
tc	1384.14	K	Joback Method
tf	782.09	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1272.59	J/mol×K	1128.75	Joback Method
cpg	1327.08	J/mol×K	1171.31	Joback Method
cpg	1387.57	J/mol×K	1213.88	Joback Method
cpg	1454.73	J/mol×K	1256.44	Joback Method
cpg	1529.24	J/mol×K	1299.01	Joback Method
cpg	1611.76	J/mol×K	1341.57	Joback Method

cpg	1702.96	J/mol×K	1384.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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