9-fluoro-11,17-dihydroxy-17-(2-hydroxyacetyl)-10,

Other names: Fludrocortisone
Inchi: InChI=1S/C21H29FO5/c1-18-7-5-13(24)9-12(18)3-4-15-14-6-8-20(27,17(26)11-23)19(14
InchiKey: AAXVEMMRQDVLJB-UHFFFAOYSA-N
Formula: C21H29FO5
SMILES: CC12CCC(=O)C=C1CCC1C3CCC(O)(C(=O)CO)C3(C)CC(O)C12F
Mol. weight [g/mol]: 380.46

Physical Properties

Property code	Value	Unit	Source
gf	-573.10	kJ/mol	Joback Method
hf	-1073.20	kJ/mol	Joback Method
hfus	27.49	kJ/mol	Joback Method
hvap	118.49	kJ/mol	Joback Method
log10ws	-3.43		Estimated Solubility Method
log10ws	-1.79		Aqueous Solubility Prediction Method
log10ws	-3.43		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.874		Crippen Method
mcvol	281.530	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	1116.78	K	Joback Method
tc	1367.43	K	Joback Method
tf	777.95	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.43	J/mol×K	1116.78	Joback Method
cpg	1271.03	J/mol×K	1158.55	Joback Method
cpg	1329.45	J/mol×K	1200.33	Joback Method
cpg	1394.35	J/mol×K	1242.10	Joback Method

cpg	1466.36	J/mol×K	1283.88	Joback Method
cpg	1546.15	J/mol×K	1325.65	Joback Method
cpg	1634.37	J/mol×K	1367.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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

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