Pregn-4-ene-3,20-dione, 9alpha-fluoro-11,17alpha,21-trihydroxy-, 21-acetate

Inchi: InChI=1S/C23H31FO6/c1-13(25)30-12-19(28)22(29)9-7-16-17-5-4-14-10-15(26)6-8-20(1

InchiKey: SYWHXTATXSMDSB-UHFFFAOYSA-N

Formula: C23H31FO6

SMILES: CC(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3(F)C(O)CC21C

Mol. weight [g/mol]: 422.49

Physical Properties

Property code	Value	Unit	Source
gf	-653.36	kJ/mol	Joback Method
hf	-1207.05	kJ/mol	Joback Method
hfus	31.37	kJ/mol	Joback Method
hvap	115.42	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.445		Crippen Method
mcvol	311.280	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
tb	1146.65	K	Joback Method
tc	1403.87	K	Joback Method
tf	811.83	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.86	J/mol×K	1146.65	Joback Method
cpg	1405.29	J/mol×K	1189.52	Joback Method
cpg	1468.90	J/mol×K	1232.39	Joback Method
cpg	1539.36	J/mol×K	1275.26	Joback Method
cpg	1617.35	J/mol×K	1318.13	Joback Method
cpg	1703.56	J/mol×K	1361.00	Joback Method
cpg	1798.65	J/mol×K	1403.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005401&Units=SI

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