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

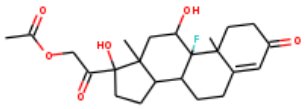
InChI: InChI=1S/C23H31FO6/c1-13(25)30-12-19(28)22(29)9-7-16-17-5-4-14-10-15(26)6-8-20(14,2)23(17,24)18(27)11-21(16,22)3/h10,16-18,27,29H,4-9,11-12H2,1-3H3

InChI Key: SYWHXTATXSMDSB-UHFFFAOYSA-N

Formula: C23H31FO6

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

Molecular Weight: 422.49



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-653.36	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1207.05	kJ/mol	Joback Method
$\Delta_{fus} H°$	31.37	kJ/mol	Joback Method
$\Delta_{vap} H°$	115.42	kJ/mol	Joback Method
$logP_{oct/wat}$	2.44		Crippen Method
P_c	1741.91	kPa	Joback Method
T_{boil}	1146.65	K	Joback Method
T_c	1403.87	K	Joback Method
T_{fus}	811.83	K	Joback Method
V_c	1.18	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1347.86	J/mol×K	1146.65	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/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(14,2)23(17,24)18(27)11-21(16,22)3/h10,16-18,27,29H,4-9,11-12H2,1-3H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).