Betamethasone-17-valerate

Other names: [9-fluoro-11-hydroxy-17-(2-hydroxyacetyl)-10,13,16-trimethyl-3-oxo-6,7,8,11,12,14,15,16-pentanoate

Inchi: InChI=1S/C27H37FO6/c1-5-6-7-23(33)34-27(22(32)15-29)16(2)12-20-19-9-8-17-13-18(3

InchiKey: SNHRLVCMMWUAJD-UHFFFAOYSA-N

Formula: C27H37FO6

SMILES: CCCCC(=O)OC1(C(=O)CO)C(C)CC2C3CCC4=CC(=O)C=CC4(C)C3(F)C(O)CC21C

Mol. weight [g/mol]: 476.58

Physical Properties

Property code	Value	Unit	Source
gf	-597.43	kJ/mol	Joback Method
hf	-1252.17	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	124.30	kJ/mol	Joback Method
log10ws	-4.71		Aqueous Solubility Prediction Method
log10ws	-4.71		Estimated Solubility Method
logp	3.637		Crippen Method
mcvol	363.340	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
tb	1232.66	K	Joback Method
tc	1519.45	K	Joback Method
tf	456.65	K	Aqueous Solubility Prediction Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1663.22	J/mol×K	1232.66	Joback Method
cpg	1743.91	J/mol×K	1280.46	Joback Method
cpg	1833.80	J/mol×K	1328.26	Joback Method
cpg	1933.84	J/mol×K	1376.05	Joback Method
cpg	2044.99	J/mol×K	1423.85	Joback Method
cpg	2168.21	J/mol×K	1471.65	Joback Method

cpg	2304.45	J/mol×K	1519.45	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
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
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