Prednisolone, 9alpha-fluoro-16alpha-methyl-, acetate

Other names: 16«alpha»-Methyl-9«alpha»-fluoroprednisolone 21-acetate

9-Fluoro-11«beta»,17,21-trihydroxy-16«alpha»-methylpregna-1,4-diene-3,20-dione 21-acetate

9«alpha»-Fluoro-16«alpha»-methylprednisolone acetate

Dalalone DP

Dalalone LA

Decadron-L.A.

Decadron-LA

Decadronal

Dectan

Dectancyl

Dex-Cortidelt acetate

Dexa-Cortisyl

Dexamethasome acetate

Dexamethasone acetate

Fortecortin

Fortecortin (crystal suspension)

NSC 39471

Panasone

Prednisolone, 9«alpha»-fluoro-16«alpha»-methyl-, acetate

Pregna-1,4-diene-3,20-dione, 21-(acetyloxy)-9-fluoro-11,17-dihydroxy-16-methyl-, (11«beta»,16«alpha»)-

Pregna-1,4-diene-3,20-dione, 9-fluoro-11«beta»,17,21-trihydroxy-16«alpha»-methyl-, 21-acetate

Pregna-1,4-diene-3,20-dione, 9-fluoro-11«beta»,17,21-trihydroxy-16«alpha»-methyl-, acetate

[2-(9-fluoro-11,17-dihydroxy-10,13,16-trimethyl-3-oxo-6,7,8,11,12,14,15,16-octahydrocyc

Inchi: InChI=1S/C24H31FO6/c1-13-9-18-17-6-5-15-10-16(27)7-8-21(15,3)23(17,25)19(28)11-2

acetate

InchiKey: AKUJBENLRBOFTD-UHFFFAOYSA-N

Formula: C24H31FO6

SMILES: CC(=O)OCC(=O)C1(O)C(C)CC2C3CCC4=CC(=O)C=CC4(C)C3(F)C(O)CC21C

Mol. weight [g/mol]: 434.50

Physical Properties

Property code	Value	Unit	Source
hfus	36.25	kJ/mol	Joback Method
log10ws	-4.90		Aqueous Solubility Prediction Method
log10ws	-4.90		Estimated Solubility Method
logp	2.466		Crippen Method

mcvol	321.070	ml/mol	McGowan Method
tf	520.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1397.32	J/mol×K	1164.02	Joback Method
cpg	1457.99	J/mol×K	1207.62	Joback Method
cpg	1525.23	J/mol×K	1251.23	Joback Method
cpg	1599.75	J/mol×K	1294.83	Joback Method
cpg	1682.25	J/mol×K	1338.43	Joback Method
cpg	1773.45	J/mol×K	1382.04	Joback Method
cpg	1874.05	J/mol×K	1425.64	Joback Method
hfust	37.72	kJ/mol	503.00	NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1177873&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point