Dexamethasone-21-acetate

Other names:

16«alpha»-Methyl-9«alpha»-fluoroprednisolone 21-acetate
16Â«alphaÂ»-Methyl-9Â«alphaÂ»-fluoroprednisolone 21-acetate
9-Fluoro-11«beta»,17,21-trihydroxy-16«alpha»-methylpregna-1,4-diene-3,20-dione 21-acetate
9-Fluoro-11Â«betaÂ»,17,21-trihydroxy-16Â«alphaÂ»-methylpregna-1,4-diene-3,20-dione 21-acetate
9«alpha»-Fluoro-16«alpha»-methylprednisolone acetate
9Â«alphaÂ»-Fluoro-16Â«alphaÂ»-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, 9alpha-fluoro-16alpha-methyl-, acetate
Prednisolone, 9«alpha»-fluoro-16«alpha»-methyl-, acetate
Prednisolone, 9Â«alphaÂ»-fluoro-16Â«alphaÂ»-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, 21-(acetyloxy)-9-fluoro-11,17-dihydroxy-16-methyl-, (11Â«betaÂ», 16Â«alphaÂ»)-
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
Pregna-1,4-diene-3,20-dione, 9-fluoro-11Â«betaÂ»,17,21-trihydroxy-16Â«alphaÂ»-methyl-, 21-acetate
Pregna-1,4-diene-3,20-dione, 9-fluoro-11Â«betaÂ»,17,21-trihydroxy-16Â«alphaÂ»-methyl-, acetate
[2-(9-fluoro-11,17-dihydroxy-10,13,16-trimethyl-3-oxo-6,7,8,11,12,14,15,16-octahydrocyc
acetate

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

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

CAS: 1177-87-3

Physical Properties

Property code	Value	Unit	Source
gf	-622.69	kJ/mol	Joback Method
hf	-1190.25	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	117.63	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
pc	1614.17	kPa	Joback Method
tb	1164.02	K	Joback Method
tc	1425.64	K	Joback Method
tf	520.65	K	Aqueous Solubility Prediction Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1773.45	J/mol×K	1382.04	Joback Method
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	1874.05	J/mol×K	1425.64	Joback Method
hfust	37.72	kJ/mol	503.00	NIST Webbook

Sources

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1177873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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