Dexamethasone

Other names:	(11.beta.,16.alpha.)-9-fluoro-11,17,21-trihydroxy-16-methylpregna-1.4-diene-3,20-dione (8S,9R,10S,11S,13S,14S,16R,17R)-9-fluoro-11,17-dihydroxy-17-(2-hydroxyacetyl)-10,13 1-dehydro-16.alpha.-methyl-9.alpha.-fluorohydrocortisone 16.alpha.-methyl-9.alpha.-fluoro-1,4-pregnadiene-11.beta.,17.alpha.,21-triol-3,20-dione 9-fluoro-11.beta.,17,21-trihydroxy-16.alpha.-methylpregna-1,4-diene-3,20-dione 9.alpha.-fluoro-16.alpha.-methylprednisolone Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-methyl-, (11«beta»,16«alpha»)- Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-methyl-, (11Â«betaÂ»,16Â«alphaÂ»)- decacortin dexacortal «delta» Â«deltaÂ»
Inchi:	InChI=1S/C22H29FO5/c1-12-8-16-15-5-4-13-9-14(25)6-7-19(13,2)21(15,23)17(26)10-20
InchiKey:	UREBDLICKHMUKA-GCMAGEFQSA-N
Formula:	C22H29FO5
SMILES:	CC1CC2C3CCC4=CC(=O)C=CC4(C)C3(F)C(O)CC2(C)C1(O)C(=O)CO
Mol. weight [g/mol]:	392.46
CAS:	50-02-2

Physical Properties

Property code	Value	Unit	Source
gf	-542.43	kJ/mol	Joback Method
hf	-1056.40	kJ/mol	Joback Method
hfus	32.38	kJ/mol	Joback Method
hvap	120.70	kJ/mol	Joback Method
log10ws	-3.59		Estimated Solubility Method
log10ws	-3.68		Aqueous Solubility Prediction Method
logp	1.896		Crippen Method
mcvol	291.320	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2970.00		NIST Webbook
tb	1134.15	K	Joback Method
tc	1389.42	K	Joback Method
tf	535.65	K	Aqueous Solubility Prediction Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1266.64	J/mol×K	1134.15	Joback Method
cpg	1322.47	J/mol×K	1176.69	Joback Method
cpg	1384.52	J/mol×K	1219.24	Joback Method
cpg	1453.49	J/mol×K	1261.78	Joback Method
cpg	1530.04	J/mol×K	1304.33	Joback Method
cpg	1614.86	J/mol×K	1346.87	Joback Method
cpg	1708.64	J/mol×K	1389.42	Joback Method
hfust	42.02	kJ/mol	539.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50022&Units=SI

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

Solubility of Dexamethasone in Supercritical Carbon Dioxide: https://www.doi.org/10.1021/je301065f

Solubility of Dexamethasone in Supercritical Carbon Dioxide with and without a Cosolvent: https://www.doi.org/10.1021/je500345n

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume