Triamcinolone

Other names:

(11«beta»,16«alpha»)-9-Fluoro-11,16,17,21-tetrahydroxypregna-1,4-diene-3,20-dione
(11Â«betaÂ»,16Â«alphaÂ»)-9-Fluoro-11,16,17,21-tetrahydroxypregna-1,4-diene-3,20-dio
11«beta»,16«alpha»,17«alpha»,21-Tetrahydroxy-9«alpha»-fluoro-1,4-pregnadiene-3,20-
11Â«betaÂ»,16Â«alphaÂ»,17Â«alphaÂ»,21-Tetrahydroxy-9Â«alphaÂ»-fluoro-1,4-pregna
9-Fluoro-11-«beta»,16-«alpha»,17,21-tetrahydroxypregna-1,4-diene-3,20-dione
9-Fluoro-11-Â«betaÂ»,16-Â«alphaÂ»,17,21-tetrahydroxypregna-1,4-diene-3,20-dione
9Alpha-fluoro-11beta,16alpha,17alpha,21-tetrahydroxypregna-1,4-diene-3,20-dione
9«alpha»-Fluoro-11«beta»,16«alpha»,17,21-tetrahydroxy-1,4-pregnadiene-3,20-dione
9«alpha»-Fluoro-11«beta»,16«alpha»,17,21-tetrahydroxypregna-1,4-diene-3,20-dione
9«alpha»-Fluoro-11«beta»,16«alpha»,17«alpha»,21-tetrahydroxypregna-1,4-diene-3,20-
9«alpha»-Fluoro-16«alpha»-hydroxyprednisolone
9Â«alphaÂ»-Fluoro-11Â«betaÂ»,16Â«alphaÂ»,17,21-tetrahydroxy-1,4-pregnadiene-3,20
9Â«alphaÂ»-Fluoro-11Â«betaÂ»,16Â«alphaÂ»,17,21-tetrahydroxypregna-1,4-diene-3,20
9Â«alphaÂ»-Fluoro-11Â«betaÂ»,16Â«alphaÂ»,17Â«alphaÂ»,21-tetrahydroxypregna-1,4-
9Â«alphaÂ»-Fluoro-16Â«alphaÂ»-hydroxyprednisolone
Adcortyl
Aristocort
CL 19823
Celeste
Cinolone
Cinolone-T
Delphicort
Fluoxiprednisolone
Fluoxyprednisolone
Kenacort
Kenacort-AG
Ledercort
Mycolog
NSC 13397
Omicilon
Polcortolon
Prednisolone, 9-fluoro-16«alpha»-hydroxy-
Prednisolone, 9-fluoro-16Â«alphaÂ»-hydroxy-
Pregna-1,4-diene-3,20-dione, 9-fluoro-11,16,17,21-tetrahydroxy-, (11«beta»,16«alpha»)-
Pregna-1,4-diene-3,20-dione, 9-fluoro-11,16,17,21-tetrahydroxy-, (11Â«betaÂ»,16Â«alphaÂ»)-
Pregna-1,4-diene-3,20-dione, 9-fluoro-11«beta»,16«alpha»,17,21-tetrahydroxy-
Pregna-1,4-diene-3,20-dione, 9-fluoro-11Â«betaÂ»,16Â«alphaÂ»,17,21-tetrahydroxy-
Rodinolone
SK-Triamcinolone
Triam-Tablinen

	Triamcet
	Triamcinlon
	Triamcinolon
	Tricortale
	Volon
Inchi:	InChI=1S/C21H27FO6/c1-18-6-5-12(24)7-11(18)3-4-13-14-8-15(25)21(28,17(27)10-23)1
InchiKey:	GFNANZIMVAIWHM-OCJWOPPKSA-N
Formula:	C21H27FO6
SMILES:	CC12C=CC(=O)C=C1CCC1C3CC(O)C(O)(C(=O)CO)C3(C)CC(O)C12F
Mol. weight [g/mol]:	394.43
CAS:	124-94-7

Physical Properties

Property code	Value	Unit	Source
gf	-687.67	kJ/mol	Joback Method
hf	-1187.99	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	135.15	kJ/mol	Joback Method
log10ws	-3.68		Estimated Solubility Method
log10ws	-3.48		Aqueous Solubility Prediction Method
logp	0.620		Crippen Method
mcvol	283.100	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
tb	1203.45	K	Joback Method
tc	1485.89	K	Joback Method
tf	835.29	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1324.59	J/mol×K	1203.45	Joback Method
cpg	1397.84	J/mol×K	1250.52	Joback Method
cpg	1480.24	J/mol×K	1297.60	Joback Method
cpg	1572.70	J/mol×K	1344.67	Joback Method

cpg	1676.14	J/mol×K	1391.75	Joback Method
cpg	1791.49	J/mol×K	1438.82	Joback Method
cpg	1919.67	J/mol×K	1485.89	Joback Method
hfust	42.56	kJ/mol	543.00	NIST Webbook
hfust	42.56	kJ/mol	543.00	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=C124947&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