CORTISONE

Other names:	11-Dehydro-17-hydroxycorticosterone
	17,21-Dihydroxypregn-4-ene-3,11,20-trione
	17-Hydroxy-11-dehydrocorticosterone
	17-hydroxy-17-(2-hydroxyacetyl)-10,13-dimethyl-1,2,6,7,8,9,12,14,15,16-decahydrocyclo
	17«alpha»,21-Dihydroxy-4-pregnene-3,11,20-trione
	17«alpha»,21«beta»-Dihydroxypregn-4-ene-3,11,20-trione
	17«alpha»-Hydroxy-11-dehydrocorticosterone
	4-Pregnene-17«alpha»,21-diol-3,11,20-trione
	Adrenalex
	Andreson
	Compound E
	Cortandren
	Cortisal
	Cortisate
	Cortisona
	Cortistal
	Cortivite
	Cortogen
	Cortone
	KE
	Kendall's Compound E
	NSC 9703
	Pregn-4-en-17«alpha»,21-diol-3,11,20-trione
	Pregn-4-ene-3,11,20-trione, 17,21-dihydroxy-
	Reichstein Fa
	Reichstein's Substance FA
	Wintersteiner's Compound F
	«DELTA»4-pregnene-17«alpha»,21-diol-3,11,20-trione
Inchi:	InChI=1S/C21H28O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2
InchiKey:	MFYSYFVPBJMHGN-YKAMNDFBSA-N
Formula:	C21H28O5
SMILES:	C[C@]12CCC(=O)C=C1CC[C@@H]1[C@@H]2C(=O)C[C@@]2(C)[C@H]1CC[C@]2(O
Mol. weight [g/mol]:	360.45

Physical Properties

Property code	Value	Unit	Source

chs	-11200.00 ± 20.00	kJ/mol	NIST Webbook
hfus	25.06	kJ/mol	Joback Method
log10ws	-3.11		Aqueous Solubility Prediction Method
log10ws	-3.11		Estimated Solubility Method
log10ws	-3.27		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.990		Crippen Method
mcvol	275.460	ml/mol	McGowan Method
tf	491.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.52	J/mol×K	1097.58	Joback Method
cpg	1176.92	J/mol×K	1139.31	Joback Method
cpg	1219.77	J/mol×K	1181.05	Joback Method
cpg	1266.54	J/mol×K	1222.78	Joback Method
cpg	1317.71	J/mol×K	1264.52	Joback Method
cpg	1373.75	J/mol×K	1306.25	Joback Method
cpg	1435.13	J/mol×K	1347.99	Joback Method
hfust	36.86	kJ/mol	495.00	NIST Webbook

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53065&Units=SI

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

Cheméo Relay (1.0):

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

Cheméo Relay (1.0, beta):

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

Legend

chs:	Standard solid enthalpy of combustion
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