Spironolactone

Other names:

17-Hydroxy-7«alpha»-mercapto-3-oxo-17«alpha»-pregn-4-ene-21-carboxylic acid «gamma»-lactone 7-acetate

17-Hydroxy-7«alpha»-mercapto-3-oxo-17«alpha»-pregn-4-ene-21-carboxylic acid «gamma»-lactone acetate

17-Hydroxy-7Â«alphaÂ»-mercapto-3-oxo-17Â«alphaÂ»-pregn-4-ene-21-carboxylic acid Â«gammaÂ»-lactone 7-acetate

17-Hydroxy-7Â«alphaÂ»-mercapto-3-oxo-17Â«alphaÂ»-pregn-4-ene-21-carboxylic acid Â«gammaÂ»-lactone acetate

17-«alpha»-Pregn-4-ene-21-carboxylic acid, 17-hydroxy-7-«alpha»-mercapto-3-oxo-«gamma»-lactone

17-Â«alphaÂ»-Pregn-4-ene-21-carboxylic acid, 17-hydroxy-7-Â«alphaÂ»-mercapto-3-oxo-Â«gammaÂ»-lactone

17«alpha»-Pregn-4-ene-21-carboxylic acid, 17-hydroxy-7«alpha»-mercapto-3-oxo-, «gamma»-lactone, acetate

17Â«alphaÂ»-Pregn-4-ene-21-carboxylic acid, 17-hydroxy-7Â«alphaÂ»-mercapto-3-oxo-, Â«gammaÂ»-lactone, acetate

3'-(3-Oxo-7-«alpha»-acetylthio-17-«beta»-hydroxyandrost-4-en-17-«beta»-yl)propionic acid lactone

3'-(3-Oxo-7-Â«alphaÂ»-acetylthio-17-Â«betaÂ»-hydroxyandrost-4-en-17-Â«betaÂ»-yl)propionic acid lactone

3-(3-Keto-7«alpha»-acetylthio-17«beta»-hydroxy-4-androsten-17«alpha»-yl)propionic acid lactone

3-(3-Keto-7Â«alphaÂ»-acetylthio-17Â«betaÂ»-hydroxy-4-androsten-17Â«alphaÂ»-yl)propionic acid lactone

3-(3-Oxo-7«alpha»-acetylthio-17«beta»-hydroxy-4-androsten-17«alpha»-yl)propionic acid-«gamma»-lactone

3-(3-Oxo-7Â«alphaÂ»-acetylthio-17Â«betaÂ»-hydroxy-4-androsten-17Â«alphaÂ»-yl)propionic acid-Â«gammaÂ»-lactone

7-«alpha»-(acetylthio)-17-«alpha»-hydroxy-3-oxopregn-4-ene-21-carboxylic acid, «gamma»-lactone

7-«alpha»-Acetylthio-3-oxo-17-«alpha»-pregn-4-ene-21,17-«beta»-carbolactone

7-Â«alphaÂ»-(acetylthio)-17-Â«alphaÂ»-hydroxy-3-oxopregn-4-ene-21-carboxylic acid, Â«gammaÂ»-lactone

7-Â«alphaÂ»-Acetylthio-3-oxo-17-Â«alphaÂ»-pregn-4-ene-21,17-Â«betaÂ»-carbolactone

Abbolactone

Acelat

Aldace

Aldactone

Aldactone A

Alderon

Aldopur

Almatol

Altex

Aquareduct

Berlactone

Deverol

Diatensec

Dira

Duraspiron

Euteberol

Lacalmin

Lacdene

Laractone

Melarcon

Nefurofan

Osiren

Osyrol

Pregn-4-ene-21-carboxylic acid, 7-(acetylthio)-17-hydroxy-3-oxo-, «gamma»-lactone, (7«alpha»,17«alpha»)-

Pregn-4-ene-21-carboxylic acid, 7-(acetylthio)-17-hydroxy-3-oxo-, Â«gammaÂ»-lactone, (7Â«alphaÂ»,17Â«alphaÂ»)-

SC 15983

SC 9420

Sagisal

Sincomen

Spiresis

Spiretic

Spiridon

Spiro-Tablinen

Spiroctan

Spiroctanie

Spiroderm

Spirolactone

Spirolakton

Spirolang

Spirolone

Spirone

Spironocompren

Spironolactone A

Supra-puren

Suracton

Uractone

Urusonin

Verospiron

Verospirone

Xenalon

Inchi: InChI=1S/C24H32O4S/c1-14(25)29-19-13-15-12-16(26)4-8-22(15,2)17-5-9-23(3)18(21(1

InchiKey: LXMSZDCAJNLERA-PJKOONHHSA-N

Formula: C24H32O4S

SMILES: CC(=O)SC1CC2=CC(=O)CCC2(C)C2CCC3(C)C(CCC34CCC(=O)O4)C12

Mol. weight [g/mol]: 416.57

CAS: 52-01-7

Physical Properties

Property code	Value	Unit	Source
gf	-56.31	kJ/mol	Joback Method
hf	-638.41	kJ/mol	Joback Method

hfus	32.80	kJ/mol	Joback Method
hvap	93.06	kJ/mol	Joback Method
log10ws	-4.17		Estimated Solubility Method
log10ws	-4.20		Aqueous Solubility Prediction Method
logp	4.852		Crippen Method
mcvol	317.350	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	3280.00		NIST Webbook
tb	1088.60	K	Joback Method
tc	1370.40	K	Joback Method
tf	481.57	K	Determination and correlation of solubility of spironolactone form II in pure solvents and binary solvent mixtures
tf	407.65	K	Aqueous Solubility Prediction Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1278.66	J/mol×K	1088.60	Joback Method
cpg	1324.26	J/mol×K	1135.57	Joback Method
cpg	1373.94	J/mol×K	1182.53	Joback Method
cpg	1428.39	J/mol×K	1229.50	Joback Method
cpg	1488.32	J/mol×K	1276.47	Joback Method
cpg	1554.45	J/mol×K	1323.43	Joback Method
cpg	1627.47	J/mol×K	1370.40	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52017&Units=SI

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

Solubility of spironolactone in supercritical carbon dioxide: Experimental and modeling approaches: https://www.doi.org/10.1016/j.fluid.2013.07.003

Determination and correlation of solubility of spironolactone form II in pure solvents and binary solvent mixtures: https://www.doi.org/10.1016/j.jct.2014.07.011

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
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