Diosgenin

Other names:	(20R,25R)-spirost-5-en-3«beta»-ol
	(20R,25R)-spirost-5-en-3Â«betaÂ»-ol
	(25R)-Spirost-5-en-3beta-ol
	(25R)-Spirost-5-en-3«beta»-ol
	(25R)-Spirost-5-en-3Â«betaÂ»-ol
	(3.beta.,25R)-spirost-5-en-3-ol
	22«alpha»-Spirost-5-en-3«beta»-ol
	22Â«alphaÂ»-Spirost-5-en-3Â«betaÂ»-ol
	25D-Spirost-5-en-3beta-ol
	25D-spirost-5-en-3«beta»-ol
	25D-spirost-5-en-3Â«betaÂ»-ol
	NSC 33396
	Nitogenin
	SP 37
	Spiro(8H-naphth(2',1':4,5)-indeno(2,1-b)furan-8,2'-(2H)-pyran)-2-ol, 1,2,3,3',4,4',4a,4b,5,5',6,6',6a,6b,7,9a,10,10a,10b,11-eicosahydro-4a,5',6a,7-tetramethyl-
	Spiro[8H-naphth[2',1':4,5]indeno[2,1-b]furan-8,2'-[2H]pyran], spirost-5-en-3-ol deriv.
	Spirost-5-en-3-ol, (3beta,25R)-
	Spirost-5-en-3-ol, (3«beta»,25R)-
	Spirost-5-en-3-ol, (3Â«betaÂ»,25R)-
	Spirost-5-en-3beta-ol, (25R)-
	Spirost-5-en-3«beta»-ol, (25R)-
	Spirost-5-en-3Â«betaÂ»-ol, (25R)-
Inchi:	InChI=1S/C27H42O3/c1-16-7-12-27(29-15-16)17(2)24-23(30-27)14-22-20-6-5-18-13-19(
InchiKey:	WQLVFSAGQJTQCK-ICPPQKBESA-N
Formula:	C27H42O3
SMILES:	CC1CCC2(OC1)OC1CC3C4CC=C5CC(O)CCC5(C)C4CCC3(C)C1C2C
Mol. weight [g/mol]:	414.62
CAS:	512-04-9

Physical Properties

Property code	Value	Unit	Source
gf	112.51	kJ/mol	Joback Method
hf	-632.83	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	98.03	kJ/mol	Joback Method
log10ws	-7.32		Estimated Solubility Method

log10ws	-2.62		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-5.37		Aqueous Solubility Prediction Method
logp	5.714		Crippen Method
mcvol	339.440	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook
tb	1015.08	K	Joback Method
tc	1258.05	K	Joback Method
tf	474.40	K	Experimental solubility of diosgenin and estriol in various solvents between T = (293.2-328.2) K
tf	478.65	K	Aqueous Solubility Prediction Method
tf	480.24	K	Application of the NRTL method to correlate solubility of diosgenin
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1396.38	J/mol×K	1015.08	Joback Method
cpg	1437.02	J/mol×K	1055.58	Joback Method
cpg	1480.32	J/mol×K	1096.07	Joback Method
cpg	1526.88	J/mol×K	1136.57	Joback Method
cpg	1577.23	J/mol×K	1177.06	Joback Method
cpg	1631.97	J/mol×K	1217.56	Joback Method
cpg	1691.64	J/mol×K	1258.05	Joback Method

Sources

Determination and correlation of the solubility for diosgenin in alcohols solvents:	https://www.doi.org/10.1016/j.jct.2012.02.002
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Application of the NRTL method to correlate solubility of diosgenin:	https://www.doi.org/10.1016/j.jct.2013.12.020
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Solubility of diosgenin in several imidazolium-based ionic liquids:	https://www.doi.org/10.1021/je5004324
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C512049&Units=SI
Solubility of diosgenin in different solvents:	https://www.doi.org/10.1016/j.jct.2011.11.009
Experimental solubility for betulin and estrone in various solvents within the temperature range T = (293.2 to 328.2) K:	https://www.doi.org/10.1016/j.jct.2016.02.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental solubility of diosgenin and estriol in various solvents between T = (293.2 328.2) K:	https://www.doi.org/10.1016/j.jct.2016.11.017
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

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