Megestrol acetate

Other names:

17-(acetyloxy)-6-methylpregna-4,6-diene-3,20-dione
17-Acetoxy-6-methylpregna-4,6-diene-3,20-dione
17-Hydroxy-6-methylpregna-4,6-diene-3,20-dione acetate
17-hydroxy-6-methylpregna-4,6-diene-3,20-dione 17-acetate
17«alpha»-Acetoxy-6-dehydro-6-methylprogesterone
17«alpha»-Acetoxy-6-methyl-4,6-pregnadiene-3,20-dione
17«alpha»-Acetoxy-6-methylpregna-4,6-diene-3,20-dione
17Â«alphaÂ»-Acetoxy-6-dehydro-6-methylprogesterone
17Â«alphaÂ»-Acetoxy-6-methyl-4,6-pregnadiene-3,20-dione
17Â«alphaÂ»-Acetoxy-6-methylpregna-4,6-diene-3,20-dione
5071
6-Dehydro-6-methyl-17«alpha»-acetoxyprogesterone
6-Dehydro-6-methyl-17Â«alphaÂ»-acetoxyprogesterone
6-Methyl-17-«alpha»-acetoxypregna-4,6-diene-3,20-dione
6-Methyl-17-Â«alphaÂ»-acetoxypregna-4,6-diene-3,20-dione
6-Methyl-17«alpha»-hydroxy-«DELTA»6-progesterone acetate
6-Methyl-17Â«alphaÂ»-hydroxy-Â«DELTAÂ»6-progesterone acetate
6-Methyl-6-dehydro-17«alpha»-acetoxyprogesterone
6-Methyl-6-dehydro-17«alpha»-acetylprogesterone
6-Methyl-6-dehydro-17Â«alphaÂ»-acetoxyprogesterone
6-Methyl-6-dehydro-17Â«alphaÂ»-acetylprogesterone
6-Methyl-«DELTA»4,6-pregnadien-17-«alpha»-ol-3,20-dione acetate
6-Methyl-Â«DELTAÂ»4,6-pregnadien-17-Â«alphaÂ»-ol-3,20-dione acetate
BDH 1298
DMAP
Magestin
Maygace
Megace
Megeron
Megestat
Megestil
Megestryl acetate
NSC-71423
Nia
Niagestin
Ovaban
Ovarid
Pregna-4,6-diene-3,20-dione, 17-(acetyloxy)-6-methyl-
Pregna-4,6-diene-3,20-dione, 17-hydroxy-6-methyl-, acetate
Progesterone, 6-dehydro-17«alpha»-hydroxy-6-methyl-, acetate

	Progesterone, 6-dehydro-17Â«alphaÂ»-hydroxy-6-methyl-, acetate
	SC 10363
Inchi:	InChI=1S/C24H32O4/c1-14-12-18-19(22(4)9-6-17(27)13-21(14)22)7-10-23(5)20(18)8-11
InchiKey:	RQZAXGRLVPAYTJ-UHFFFAOYSA-N
Formula:	C24H32O4
SMILES:	CC(=O)OC1(C(C)=O)CCC2C3C=C(C)C4=CC(=O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	384.51
CAS:	595-33-5

Physical Properties

Property code	Value	Unit	Source
gf	-142.96	kJ/mol	Joback Method
hf	-675.71	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	87.52	kJ/mol	Joback Method
log10ws	-5.35		Aqueous Solubility Prediction Method
log10ws	-5.35		Estimated Solubility Method
logp	4.575		Crippen Method
mcvol	307.560	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2909.00		NIST Webbook
rinpol	2909.00		NIST Webbook
tb	994.47	K	Joback Method
tc	1245.97	K	Joback Method
tf	694.49	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.19	J/mol×K	994.47	Joback Method
cpg	1177.87	J/mol×K	1036.39	Joback Method
cpg	1214.85	J/mol×K	1078.30	Joback Method
cpg	1254.63	J/mol×K	1120.22	Joback Method
cpg	1297.72	J/mol×K	1162.14	Joback Method

cpg	1344.61	J/mol×K	1204.06	Joback Method
cpg	1395.81	J/mol×K	1245.97	Joback Method

Sources

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=C595335&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of megestrol acetate and levonorgestrel in supercriticalcarbon dioxide:	https://www.doi.org/10.1016/j.tca.2013.07.018
Solubility of Bicalutamide, Megestrol Acetate, Prednisolone, Beclomethasone Dipropionate, and Clarithromycin in Subcritical Water at Different Temperatures from 383.15 to 443.15 K:	https://www.doi.org/10.1021/acs.jced.6b00997
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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