Ethynodiol diacetate

Other names: 19-Norpregn-4-en-20-yne-3,17-diol, diacetate, (3«beta»,17«alpha»)-
19-Nor-17-«alpha»-pregn-4-en-20-yne-3-«beta»,17-diol diacetate
8080 C. B.
Cervicundin
3«beta», 17«beta»-Diacetoxy-17-«alpha»-ethynyl-4-oestrene
3«beta»,17«beta»-Diacetoxy-19-nor-17-«alpha»-pregn-4-en-20-yne
Ethinodiol diacetate
Ethynodiol acetate
«beta»-Ethynodiol diacetate
17«alpha»-Ethynyl-3,17-dihydroxy-4-estrene diacetate, (3«beta»,17«beta»)-
17«alpha»-Ethynylestr-4-ene-3«beta»,17«beta»-diol acetate
17«alpha»-Ethynyl-4-estrene-3«beta»,17«beta»-diol diacetate
17«alpha»-Ethynyl-4-estrene-3«beta»,17-diol diacetate
17«alpha»-Ethynyl-19-norandrost-4-ene-3«beta»,17«beta»-diol diacetate
Femulen
Luto-metrodiol
Metrodiol
Metrodiol diacetate
(3-«beta»,17-«alpha»)-19-Norpregn-4-en-20-yne-3,17-diol diacetate
Ovulen 50
SC 11800
19-Nor-17«alpha»-pregn-4-en-20-yn-3«beta»,17-diol diacetate
Luteonorm
Etynodiol diacetate

Inchi: InChI=1S/C24H32O4/c1-5-24(28-16(3)26)13-11-22-21-8-6-17-14-18(27-15(2)25)7-9-19(1

InchiKey: ONKUMRGIYFNPJW-AIQDNJDKSA-N

Formula: C24H32O4

SMILES: C#CC1(OC(C)=O)CCC2C3CCC4=CC(OC(C)=O)CCC4C3CCC21C

Mol. weight [g/mol]: 384.51

CAS: 297-76-7

Physical Properties

Property code	Value	Unit	Source
gf	75.15	kJ/mol	Joback Method
hf	-460.22	kJ/mol	Joback Method
hfus	39.95	kJ/mol	Joback Method

hvap	85.42	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.426		Crippen Method
mcvol	307.560	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
tb	930.14	K	Joback Method
tc	1172.80	K	Joback Method
tf	654.05	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.61	J/mol×K	930.14	Joback Method
cpg	1122.89	J/mol×K	970.58	Joback Method
cpg	1150.65	J/mol×K	1011.03	Joback Method
cpg	1179.23	J/mol×K	1051.47	Joback Method
cpg	1209.00	J/mol×K	1091.92	Joback Method
cpg	1240.33	J/mol×K	1132.36	Joback Method
cpg	1273.56	J/mol×K	1172.80	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C297767&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
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