

Mestranol

Other names:	19-Norpregna-1,3,5(10)-trien-20-yn-17-ol, 3-methoxy-, (17«alpha»)- 19-Nor-17«alpha»-pregna-1,3,5(10)-trien-20-yn-17-ol, 3-methoxy- «delta»-MVE Devocin Ethinylestradiol methyl ether Ethinylestradiol 3-methyl ether EE 3ME Inostral Norquen Ovastol 17«alpha»-Ethinylestradiol 3-Methyl ether 17«alpha»-Ethinylestradiol 3-methyl ether 17-Ethinylestradiol 3-methyl ether 3-Methoxy-17«alpha»-ethinylestradiol 3-Methoxyethinylestradiol 3-O-Methylethinylestradiol (+)-17«alpha»-Ethinyl-17«beta»-hydroxy-3-methoxy-1,3,5(10)-estratriene (+)-17«alpha»-Ethinyl-17«beta»-hydroxy-3-methoxy-1,3,5(10)-oestratriene Estra-1,3,5(10)-trien-17«beta»-ol, 17-ethinyl-3-methoxy- Ethinyloestradiol 3-methyl ether Ethinyloestradiol 3-methyl ether 17«alpha»-Ethinyl oestradiol 3-methyl ether 17«alpha»-Ethinyl-3-methoxy-17«beta»-hydroxy-«DELTA»1,3,5(10)-estratriene 17«alpha»-Ethinyl-3-methoxy-17«beta»-hydroxy-«DELTA»1,3,5(10)-oestratriene 17«alpha»-Ethinyloestradiol 3-methyl ether 17«alpha»-19-Norpregna-1,3,5(10)-trien-20-yn-17-ol, 3-methoxy- 17-Ethinyl-3-methoxy-1,3,5(10)-estratrien-17«beta»-ol 17-Ethinyl-3-methoxy-1,3,5(10)-oestratrien-17«beta»-ol 3-Methoxy-17«alpha»-ethinyloestradiol 3-Methoxy-17«alpha»-ethinyl-1,3,5(10)-estratrien-17«beta»-ol 3-Methoxy-17«alpha»-ethinyl-1,3,5(10)-oestratrien-17«beta»-ol 3-Methoxy-17«alpha»-ethinyloestradiol 3-Methoxy-19-nor-17«alpha»-pregna-1,3,5(10)-trien-20-yn-17-ol 3,17-«beta»-Dihydroxy-17-«alpha»-ethinyl-1,3,5(10)-estratriene-3-methyl ether Estra-1,3,5(10)-trien-17-«beta»-ol, 17-«alpha»-ethinyl-3-methoxy- 17-«alpha»-Ethinyl-3-methoxy-1,3,5(10)-estratrien-17-«beta»-ol 17«alpha»-Ethinyloestradiol methyl ether 17-Ethinyloestradiol 3-methyl ether 3-Methoxyethinyloestradiol 3-Methoxy-17-ethinyloestradiol-17-«beta»
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Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

3-Methoxy-17-«alpha»-19-norpregna-1,3,5(10)-trien-20-yn-17-ol

(17-«alpha»)-3-METHOXY-19-NORPREGNA-1,3,5(10)-TRIEN-20-YN-17-OL

3-Methylethynyloestradiol

3-Methoxy-19-nor-17«alpha»-pregna-1,3,5(10)-trien-20-yn-17«beta»-ol

Menophase

3-Methoxy-19-norpregna-1,3,5(10)-trien-20-yn-17-ol (mestranol)

InChI=1S/C21H26O2/c1-4-21(22)12-10-19-18-7-5-14-13-15(23-3)6-8-16(14)17(18)9-11-2

IMSSROKUHAOUJS-ALAWOQLPSA-N

C21H26O2

C#CC1(O)CCC2C3CCc4cc(OC)ccc4C3CCC21C

310.43

72-33-3

Physical Properties

Property code	Value	Unit	Source
gf	331.99	kJ/mol	Joback Method
hf	-59.85	kJ/mol	Joback Method
hfus	31.41	kJ/mol	Joback Method
hvap	82.05	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.916		Crippen Method
mcvol	253.550	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	841.14	K	Joback Method
tc	1075.44	K	Joback Method
tf	427.00 ± 1.00	K	NIST Webbook
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.27	J/mol×K	841.14	Joback Method
cpg	857.34	J/mol×K	880.19	Joback Method
cpg	879.70	J/mol×K	919.24	Joback Method
cpg	902.71	J/mol×K	958.29	Joback Method

cpg	926.69	J/mol×K	997.34	Joback Method
cpg	952.01	J/mol×K	1036.39	Joback Method
cpg	978.99	J/mol×K	1075.44	Joback Method
hfust	34.55	kJ/mol	424.10	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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