Norethynodrel

Other names:	19-Norpregn-5(10)-en-20-yn-3-one, 17-hydroxy-, (17«alpha»)-
	Enidrel
	Estr-5(10)-en-3-one, 17«alpha»-ethynyl-17-hydroxy-
	Norethinodrel
	Norethinynodrel
	Norethynodral
	SC-4642
	17«alpha»-Ethinyl-«DELTA»5(10)-19-nortestosterone
	17«alpha»-Ethinyl-estra(5,10)eneolone
	17«alpha»-Ethinyl-17«beta»-hydroxy-«DELTA»5(10)-estren-3-one
	17«alpha»-Ethinyl-5,10-estrenolone
	17«alpha»-Ethynyl-estr-5(10)-en-3-on-17«beta»-ol
	17«alpha»-Ethynyl-17«beta»-hydroxy-«DELTA»5(10)-estren-3-one
	17«alpha»-Ethynyl-17«beta»-hydroxy-3-oxo-«DELTA»5(10)-estrene
	17«alpha»-Ethynyl-17«beta»-hydroxyestr-5(10)-en-3-one
	17«alpha»-Ethynyl-17-hydroxy-5(10)-estren-3-one
	17«alpha»-Ethynyl-19-nor-5(10)-androsten-17«beta»-ol-3-one
	17«alpha»-Ethynyl-5(10)-estren-17-ol-3-one
	17«alpha»-Ethynylestr-5(10)-en-17«beta»-ol-3-one
	17-Hydroxy(17«alpha»)-19-norpregn-5(10)-en-20-yn-3-one
	17-Hydroxy-19-nor-17«alpha»-pregn-5(10)-en-20-yn-3-one
	19-nor-17«alpha»-Pregn-5(10)-en-20-yn-3-one, 17-hydroxy-
	19-Norethynodrel
	17-Ethinyl-5(10)-estraeneolone
	17-«alpha»-Ethynyl-17-hydroxyestr-5(10)-en-3-one
	17-«alpha»-Ethynyl-17-«beta»-hydroxy-5(10)-estren-3-one
	(17-«alpha»)-17-Hydroxy-19-norpregn-5(10)-en-20-yn-3-one
	17-«beta»-Hydroxy-17-«alpha»-ethinyl-5(10)-estren-3-one
	Lynestrol
	19-Nor-ethinyl-5,10-testosterone
	NSC-15432
	Noretynodrel
	17«alpha»-Hydroxy-19-norpregn-5(10)-en-20-yn-3-one
	17-Ethynyl-17-hydroxyestr-«DELTA»5(10)-en-3-one, (17«alpha»,17«beta»)-
	5(10)-Estren-3-one, 17alpha-ethynyl-17beta-hydroxy-
Inchi:	InChI=1S/C20H26O2/c1-3-20(22)11-9-18-17-6-4-13-12-14(21)5-7-15(13)16(17)8-10-19(1
InchiKey:	ICTXHFFSOAJUMG-CEVCPLMDSA-N
Formula:	C20H26O2
SMILES:	C#CC1(O)CCC2C3CCC4=C(CCC(=O)C4)C3CCC21C
Mol. weight [g/mol]:	298.42

CAS: 68-23-5

Physical Properties

Property code	Value	Unit	Source
gf	255.69	kJ/mol	Joback Method
hf	-148.78	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	80.41	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.637		Crippen Method
mcvol	243.760	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	860.36	K	Joback Method
tc	1106.20	K	Joback Method
tf	614.69	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.60	J/mol×K	860.36	Joback Method
cpg	863.44	J/mol×K	901.33	Joback Method
cpg	887.64	J/mol×K	942.31	Joback Method
cpg	912.58	J/mol×K	983.28	Joback Method
cpg	938.63	J/mol×K	1024.25	Joback Method
cpg	966.17	J/mol×K	1065.23	Joback Method
cpg	995.57	J/mol×K	1106.20	Joback Method

Sources

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=C68235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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