

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
Ethynylestradiol methyl ether
Ethynylestradiol 3-methyl ether
EE 3ME
Inostral
Norquen
Ovastol
17«alpha»-Ethinylestradiol 3-Methyl ether
17«alpha»-Ethynylestradiol 3-methyl ether
17-Ethynylestradiol 3-methyl ether
3-Methoxy-17«alpha»-ethynylestradiol
3-Methoxyethynylestradiol
3-O-Methylethynylestradiol
(+)-17«alpha»-Ethynyl-17«beta»-hydroxy-3-methoxy-1,3,5(10)-estratriene
(+)-17«alpha»-Ethynyl-17«beta»-hydroxy-3-methoxy-1,3,5(10)-oestratriene
Estra-1,3,5(10)-trien-17«beta»-ol, 17-ethynyl-3-methoxy-
Ethynloestradiol 3-methyl ether
Ethynyloestradiol 3-methyl ether
17«alpha»-Ethinyl oestradiol 3-methyl ether
17«alpha»-Ethynyl-3-methoxy-17«beta»-hydroxy-«DELTA»1,3,5(10)-estratriene
17«alpha»-Ethynyl-3-methoxy-17«beta»-hydroxy-«DELTA»1,3,5(10)-oestratriene
17«alpha»-Ethynyloestradiol 3-methyl ether
17«alpha»-19-Norpregna-1,3,5(10)-trien-20-yn-17-ol, 3-methoxy-
17-Ethynyl-3-methoxy-1,3,5(10)-estratrien-17«beta»-ol
17-Ethynyl-3-methoxy-1,3,5(10)-oestratrien-17«beta»-ol
3-Methoxy-17«alpha»-ethynloestradiol
3-Methoxy-17«alpha»-ethynyl-1,3,5(10)-estratrien-17«beta»-ol
3-Methoxy-17«alpha»-ethynyl-1,3,5(10)-oestratrien-17«beta»-ol
3-Methoxy-17«alpha»-ethynyloestradiol
3-Methoxy-19-nor-17«alpha»-pregna-1,3,5(10)-trien-20-yn-17-ol
3,17-«beta»-Dihydroxy-17-«alpha»-ethynyl-1,3,5(10)-estratriene-3-methyl ether
Estra-1,3,5(10)-trien-17-«beta»-ol, 17-«alpha»-ethynyl-3-methoxy-
17-«alpha»-Ethynyl-3-methoxy-1,3,5(10)-estratrien-17-«beta»-ol
17«alpha»-Ethynyloestradiol methyl ether
17-Ethynyloestradiol 3-methyl ether
3-Methoxyethynyloestradiol
3-Methoxy-17-ethynyloestradiol-17-«beta»

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-Methylethyloestradiol
 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)

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|----------------------|---|--|--|
| Inchi: | 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 | | |
| InchiKey: | IMSSROKUHAOUJS-ALAWOQLPSA-N | | |
| Formula: | C21H26O2 | | |
| SMILES: | C#CC1(O)CCC2C3CCc4cc(OC)ccc4C3CCC21C | | |
| Mol. weight [g/mol]: | 310.43 | | |
| CAS: | 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

| | |
|------------------------|---|
| 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/ci9903071 |
| 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 |
| 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 |
| 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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