# Dienestrol

**Other names:**

2,4-Hexadiene, 3,4-bis(4-hydroxyphenyl)-
3,4-Bis(4-hydroxyphenyl)-2,4-hexadiene
3,4-Bis(p-hydroxyphenyl)-2,4-hexadiene
4,4'-(1,2-Diethylidene-1,2-ethanediyl)bisphenol
4,4'-(Diethylideneethylene)diphenol
4,4'-Dihydroxy-«gamma»,«delta»-diphenyl-«beta»,«delta»-hexadiene
4,4'-Dihydroxy-Â«gammaÂ»,Â«deltaÂ»-diphenyl-Â«betaÂ»,Â«deltaÂ»-hexadiene
Agaldog
Cycladiene
DV
Dehydrostilbestrol
Dehydrostilboestrol
Di(p-oxyphenyl)-2,4-hexadiene
Dienesterol
Dienoestrol
Dienoestrol bp
Dienol
Dinestrol
Dinovex
Estragard
Estraguard
Estrodienol
Estroral
Follidiene
Follormon
Gynefollin
Hormofemin
NSC 59809
Oestrasid
Oestrodiene
Oestrodienol
Oestroral
Oestrovis
Phenol, 4,4'-(1,2-diethylidene-1,2-ethanediyl)bis-
Phenol, 4,4'-(diethylideneethylene)di-
Restrol
Retalon
Sexadien
Synestrol
Teserene

| | |
|---|---|
| | Willnestrol |
| | p,p'-(Diethylideneethylene)diphenol |
| | para-Dien |
| **Inchi:** | InChI=1S/C18H18O2/c1-3-17(13-5-9-15(19)10-6-13)18(4-2)14-7-11-16(20)12-8-14/h3-12 |
| **InchiKey:** | NFDFQCUYFHCNBW-SCGPFSFSSA-N |
| **Formula:** | C18H18O2 |
| **SMILES:** | CC=C(C(=CC)c1ccc(O)cc1)c1ccc(O)cc1 |
| **Mol. weight [g/mol]:** | 266.33 |
| **CAS:** | 84-17-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 159.60 | kJ/mol | Joback Method |
| hf | -81.55 | kJ/mol | Joback Method |
| hfus | 39.81 | kJ/mol | Joback Method |
| hvap | 86.32 | kJ/mol | Joback Method |
| log10ws | -4.95 | | Aqueous Solubility Prediction Method |
| log10ws | -4.95 | | Estimated Solubility Method |
| logp | 4.605 | | Crippen Method |
| mcvol | 220.100 | ml/mol | McGowan Method |
| pc | 2853.57 | kPa | Joback Method |
| tb | 833.92 | K | Joback Method |
| tc | 1094.51 | K | Joback Method |
| tf | 500.65 | K | Aqueous Solubility Prediction Method |
| vc | 0.722 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 636.41 | J/mol×K | 833.92 | Joback Method |
| cpg | 651.62 | J/mol×K | 877.35 | Joback Method |
| cpg | 666.55 | J/mol×K | 920.78 | Joback Method |
| cpg | 681.50 | J/mol×K | 964.22 | Joback Method |
| cpg | 696.78 | J/mol×K | 1007.65 | Joback Method |
| cpg | 712.69 | J/mol×K | 1051.08 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 729.53 | J/mol×K | 1094.51 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C84173&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **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 |

# 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 |