# Estra-1,3,5(10)-trien-17«beta»-ol

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|---|---|
| **Other names:** | Estra-1,3,5(10)-trien-17-ol, (17«beta»)-<br>Estradiol, 3-deoxy-<br>1,3,5(10)-Estratriene-17«beta»-ol<br>17«beta»-Estradiol, 3-deoxy-<br>17«beta»-Hydroxyestra-1,3,5(10)-triene<br>3-Deoxy-17«beta»-estradiol<br>3-Deoxyestradiol<br>Desoxy-dihydroestrone<br>1,3,5(10)-Oestratrien-17«beta»-ol |
| **Inchi:** | InChI=1S/C18H24O/c1-18-11-10-14-13-5-3-2-4-12(13)6-7-15(14)16(18)8-9-17(18)19/h2- |
| **InchiKey:** | MUENRDYXOADTOC-UHFFFAOYSA-N |
| **Formula:** | C18H24O |
| **SMILES:** | CC12CCC3c4ccccc4CCC3C1CCC2O |
| **Mol. weight [g/mol]:** | 256.38 |
| **CAS:** | 2529-64-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 203.78 | kJ/mol | Joback Method |
| hf | -161.38 | kJ/mol | Joback Method |
| hfus | 26.17 | kJ/mol | Joback Method |
| hvap | 73.59 | kJ/mol | Joback Method |
| log10ws | -4.72 | | Crippen Method |
| logp | 3.904 | | Crippen Method |
| mcvol | 214.010 | ml/mol | McGowan Method |
| pc | 2227.09 | kPa | Joback Method |
| rinpol | 2300.00 | | NIST Webbook |
| rinpol | 2218.00 | | NIST Webbook |
| rinpol | 2218.00 | | NIST Webbook |
| tb | 754.74 | K | Joback Method |
| tc | 982.16 | K | Joback Method |
| tf | 454.58 | K | Joback Method |
| vc | 0.805 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 688.46 | J/mol×K | 754.74 | Joback Method |
| cpg | 708.37 | J/mol×K | 792.64 | Joback Method |
| cpg | 727.45 | J/mol×K | 830.55 | Joback Method |
| cpg | 745.92 | J/mol×K | 868.45 | Joback Method |
| cpg | 764.01 | J/mol×K | 906.35 | Joback Method |
| cpg | 781.94 | J/mol×K | 944.26 | Joback Method |
| cpg | 799.93 | J/mol×K | 982.16 | Joback Method |

# Sources

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|---|---|
| **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=C2529648&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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| **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 |