# 17-epi-Methandriol

**Inchi:** InChI=1S/C20H32O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(1
**InchiKey:** WRWBCPJQPDHXTJ-RZNHXTIWSA-N
**Formula:** C20H32O2
**SMILES:** CC12CCC(O)CC1=CCC1C2CCC2(C)C1CCC2(C)O
**Mol. weight [g/mol]:** 304.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 7.11 | kJ/mol | Joback Method |
| hf | -469.18 | kJ/mol | Joback Method |
| hfus | 22.92 | kJ/mol | Joback Method |
| hvap | 90.56 | kJ/mol | Joback Method |
| log10ws | -5.17 | | Crippen Method |
| logp | 4.061 | | Crippen Method |
| mcvol | 256.660 | ml/mol | McGowan Method |
| pc | 1971.80 | kPa | Joback Method |
| rinpol | 2562.00 | | NIST Webbook |
| rinpol | 2562.00 | | NIST Webbook |
| tb | 880.52 | K | Joback Method |
| tc | 1100.10 | K | Joback Method |
| tf | 563.22 | K | Joback Method |
| vc | 0.959 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 935.87 | J/mol×K | 880.52 | Joback Method |
| cpg | 961.45 | J/mol×K | 917.12 | Joback Method |
| cpg | 988.11 | J/mol×K | 953.71 | Joback Method |
| cpg | 1016.23 | J/mol×K | 990.31 | Joback Method |
| cpg | 1046.18 | J/mol×K | 1026.91 | Joback Method |
| cpg | 1078.34 | J/mol×K | 1063.51 | Joback Method |
| cpg | 1113.10 | J/mol×K | 1100.10 | 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=R257831&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 |

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