# 20«beta»,21-Dihydroxypregn-4-en-3-one, 20,21-acetonide

**Inchi:** InChI=1S/C24H36O3/c1-22(2)26-14-21(27-22)20-8-7-18-17-6-5-15-13-16(25)9-11-23(15

**InchiKey:** LIVZAOOCWISZFK-LGYJOKLQSA-N

**Formula:** C24H36O3

**SMILES:** CC1(C)OCC(C2CCC3C4CCC5=CC(=O)CCC5(C)C4CCC23C)O1

**Mol. weight [g/mol]:** 372.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 56.15 | kJ/mol | Joback Method |
| hf | -588.50 | kJ/mol | Joback Method |
| hfus | 34.51 | kJ/mol | Joback Method |
| hvap | 79.63 | kJ/mol | Joback Method |
| log10ws | -5.92 | | Crippen Method |
| logp | 5.286 | | Crippen Method |
| mcvol | 303.730 | ml/mol | McGowan Method |
| pc | 1453.46 | kPa | Joback Method |
| rinpol | 2890.00 | | NIST Webbook |
| rinpol | 2890.00 | | NIST Webbook |
| tb | 924.68 | K | Joback Method |
| tc | 1185.57 | K | Joback Method |
| tf | 618.92 | K | Joback Method |
| vc | 1.135 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1152.02 | J/mol×K | 924.68 | Joback Method |
| cpg | 1187.52 | J/mol×K | 968.16 | Joback Method |
| cpg | 1224.55 | J/mol×K | 1011.64 | Joback Method |
| cpg | 1263.72 | J/mol×K | 1055.13 | Joback Method |
| cpg | 1305.62 | J/mol×K | 1098.61 | Joback Method |
| cpg | 1350.85 | J/mol×K | 1142.09 | Joback Method |
| cpg | 1400.03 | J/mol×K | 1185.57 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R525109&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |