# Propranolol desamino dihydroxy, acetylated

**Inchi:** InChI=1S/C19H20O7/c1-12(20)23-10-15(25-13(2)21)11-24-18-8-9-19(26-14(3)22)17-7-5
**InchiKey:** LTWMZJHVSANJRJ-UHFFFAOYSA-N
**Formula:** C19H20O7
**SMILES:** CC(=O)OCC(COc1ccc(OC(C)=O)c2ccccc12)OC(C)=O
**Mol. weight [g/mol]:** 360.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -500.30 | kJ/mol | Joback Method |
| hf | -902.73 | kJ/mol | Joback Method |
| hfus | 41.27 | kJ/mol | Joback Method |
| hvap | 92.62 | kJ/mol | Joback Method |
| log10ws | -4.06 | | Crippen Method |
| logp | 2.639 | | Crippen Method |
| mcvol | 263.540 | ml/mol | McGowan Method |
| pc | 1784.86 | kPa | Joback Method |
| rinpol | 2565.00 | | NIST Webbook |
| rinpol | 2565.00 | | NIST Webbook |
| tb | 940.59 | K | Joback Method |
| tc | 1165.36 | K | Joback Method |
| tf | 611.76 | K | Joback Method |
| vc | 0.998 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 808.79 | J/mol×K | 940.59 | Joback Method |
| cpg | 819.88 | J/mol×K | 978.05 | Joback Method |
| cpg | 829.64 | J/mol×K | 1015.51 | Joback Method |
| cpg | 838.08 | J/mol×K | 1052.98 | Joback Method |
| cpg | 845.21 | J/mol×K | 1090.44 | Joback Method |
| cpg | 851.03 | J/mol×K | 1127.90 | Joback Method |
| cpg | 855.55 | J/mol×K | 1165.36 | Joback Method |
| dvisc | 0.0003559 | Pa×s | 611.76 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002379 | Pa×s | 666.56 | Joback Method |
| dvisc | 0.0001690 | Pa×s | 721.37 | Joback Method |
| dvisc | 0.0001260 | Pa×s | 776.17 | Joback Method |
| dvisc | 0.0000977 | Pa×s | 830.98 | Joback Method |
| dvisc | 0.0000782 | Pa×s | 885.78 | Joback Method |
| dvisc | 0.0000642 | Pa×s | 940.59 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R582979&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 |
| **dvisc:** | Dynamic viscosity |
| **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 |