# 5-Hydroxy-2-(4-hydroxyphenyl)-4-oxo-3,4-dihydro
# 6-o-(6-deoxyhexopyranosyl)hexopyranoside

**Inchi:** InChI=1S/C27H32O14/c1-10-20(31)22(33)24(35)26(38-10)37-9-18-21(32)23(34)25(36)27

**InchiKey:** HXTFHSYLYXVTHC-ULGGMRSYSA-N

**Formula:** C27H32O14

**SMILES:** CC1OC(OCC2OC(Oc3cc(O)c4c(c3)OC(c3ccc(O)cc3)CC4=O)C(O)C(O)C2O)C(O)C(O)C

**Mol. weight [g/mol]:** 580.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1303.22 | kJ/mol | Joback Method |
| hf | -2204.07 | kJ/mol | Joback Method |
| hfus | 103.18 | kJ/mol | Joback Method |
| hvap | 228.74 | kJ/mol | Joback Method |
| log10ws | -2.78 | | Crippen Method |
| logp | -1.165 | | Crippen Method |
| mcvol | 389.070 | ml/mol | McGowan Method |
| pc | 2372.59 | kPa | Joback Method |
| tb | 1801.06 | K | Joback Method |
| tc | 2789.49 | K | Joback Method |
| tf | 1247.94 | K | Joback Method |
| vc | 1.290 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1520.96 | J/mol×K | 1801.06 | Joback Method |
| cpg | 1499.38 | J/mol×K | 1965.80 | Joback Method |
| cpg | 1479.15 | J/mol×K | 2130.54 | Joback Method |
| cpg | 1466.96 | J/mol×K | 2295.28 | Joback Method |
| cpg | 1469.56 | J/mol×K | 2460.02 | Joback Method |
| cpg | 1493.65 | J/mol×K | 2624.75 | Joback Method |
| cpg | 1545.96 | J/mol×K | 2789.49 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=B6007557&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |