# 3-O-Acetyl-1,4-anhydro-2,5-di-O-methyl-L-fucitol

**Inchi:** InChI=1S/C10H18O5/c1-6(12-3)9-10(15-7(2)11)8(13-4)5-14-9/h6,8-10H,5H2,1-4H3
**InchiKey:** WMRPGFBDYSHQRH-UHFFFAOYSA-N
**Formula:** C10H18O5
**SMILES:** COC(C)C1OCC(OC)C1OC(C)=O
**Mol. weight [g/mol]:** 218.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -478.03 | kJ/mol | Joback Method |
| hf | -876.45 | kJ/mol | Joback Method |
| hfus | 27.35 | kJ/mol | Joback Method |
| hvap | 55.59 | kJ/mol | Joback Method |
| log10ws | -0.47 | | Crippen Method |
| logp | 0.367 | | Crippen Method |
| mcvol | 165.950 | ml/mol | McGowan Method |
| pc | 2372.59 | kPa | Joback Method |
| rinpol | 1355.88 | | NIST Webbook |
| rinpol | 1355.88 | | NIST Webbook |
| tb | 581.78 | K | Joback Method |
| tc | 779.20 | K | Joback Method |
| tf | 333.07 | K | Joback Method |
| vc | 0.610 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 443.42 | J/mol×K | 581.78 | Joback Method |
| cpg | 460.23 | J/mol×K | 614.68 | Joback Method |
| cpg | 476.29 | J/mol×K | 647.59 | Joback Method |
| cpg | 491.58 | J/mol×K | 680.49 | Joback Method |
| cpg | 506.10 | J/mol×K | 713.40 | Joback Method |
| cpg | 519.81 | J/mol×K | 746.30 | Joback Method |
| cpg | 532.69 | J/mol×K | 779.20 | Joback Method |
| dvisc | 0.0017061 | Pa×s | 333.07 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0010211 | Pa×s | 374.52 | Joback Method |
| dvisc | 0.0006770 | Pa×s | 415.97 | Joback Method |
| dvisc | 0.0004835 | Pa×s | 457.42 | Joback Method |
| dvisc | 0.0003652 | Pa×s | 498.88 | Joback Method |
| dvisc | 0.0002880 | Pa×s | 540.33 | Joback Method |
| dvisc | 0.0002349 | Pa×s | 581.78 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357236&Units=SI |

# Legend

| | |
|---|---|
| **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 |