

3,5-Di-O-acetyl-1,4-anhydro-2-O-methyl-L-fucitol

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|-----------------------------|--|
| Inchi: | InChI=1S/C11H18O6/c1-6(16-7(2)12)10-11(17-8(3)13)9(14-4)5-15-10/h6,9-11H,5H2,1-4 |
| InchiKey: | JEANRGASWOHZTF-UHFFFAOYSA-N |
| Formula: | C11H18O6 |
| SMILES: | COC1COC(C(C)OC(C)=O)C1OC(C)=O |
| Mol. weight [g/mol]: | 246.26 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -598.53 | kJ/mol | Joback Method |
| hf | -1009.67 | kJ/mol | Joback Method |
| hfus | 31.54 | kJ/mol | Joback Method |
| hvap | 64.56 | kJ/mol | Joback Method |
| log10ws | -0.67 | | Crippen Method |
| logp | 0.283 | | Crippen Method |
| mcvol | 181.610 | ml/mol | McGowan Method |
| pc | 2298.11 | kPa | Joback Method |
| rinsol | 1502.49 | | NIST Webbook |
| tb | 658.53 | K | Joback Method |
| tc | 860.46 | K | Joback Method |
| tf | 394.27 | K | Joback Method |
| vc | 0.671 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 517.37 | J/molxK | 658.53 | Joback Method |
| cpg | 533.50 | J/molxK | 692.19 | Joback Method |
| cpg | 548.74 | J/molxK | 725.84 | Joback Method |
| cpg | 563.07 | J/molxK | 759.50 | Joback Method |
| cpg | 576.46 | J/molxK | 793.15 | Joback Method |
| cpg | 588.90 | J/molxK | 826.81 | Joback Method |
| cpg | 600.36 | J/molxK | 860.46 | Joback Method |
| dvisc | 0.0015656 | Paxs | 394.27 | Joback Method |
| dvisc | 0.0009684 | Paxs | 438.31 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006539 | Paxs | 482.36 | Joback Method |
| dvisc | 0.0004715 | Paxs | 526.40 | Joback Method |
| dvisc | 0.0003576 | Paxs | 570.44 | Joback Method |
| dvisc | 0.0002822 | Paxs | 614.49 | Joback Method |
| dvisc | 0.0002298 | Paxs | 658.53 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U357240&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 |

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