

Glucose, 3-methyl, acetylated

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C15H22O10/c1-7(16)21-6-11-12(22-8(2)17)13(20-5)14(23-9(3)18)15(25-11)24 |
| InchiKey: | DCJXMAVPDMWIOR-RMEBNNNOSA-N |
| Formula: | C15H22O10 |
| SMILES: | <chem>COC1C(OC(C)=O)C(COC(C)=O)OC(OC(C)=O)C1OC(C)=O</chem> |
| Mol. weight [g/mol]: | 362.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -1057.77 | kJ/mol | Joback Method |
| hf | -1623.39 | kJ/mol | Joback Method |
| hfus | 51.04 | kJ/mol | Joback Method |
| hvap | 91.72 | kJ/mol | Joback Method |
| log10ws | -0.68 | | Crippen Method |
| logp | -0.284 | | Crippen Method |
| mvol | 252.850 | ml/mol | McGowan Method |
| pc | 1697.70 | kPa | Joback Method |
| rinpol | 2201.00 | | NIST Webbook |
| rinpol | 2201.00 | | NIST Webbook |
| tb | 898.00 | K | Joback Method |
| tc | 1109.52 | K | Joback Method |
| tf | 586.67 | K | Joback Method |
| vc | 0.940 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 841.38 | J/molxK | 898.00 | Joback Method |
| cpg | 886.01 | J/molxK | 1074.27 | Joback Method |
| cpg | 880.94 | J/molxK | 1039.01 | Joback Method |
| cpg | 873.87 | J/molxK | 1003.76 | Joback Method |
| cpg | 864.88 | J/molxK | 968.51 | Joback Method |
| cpg | 854.02 | J/molxK | 933.25 | Joback Method |
| cpg | 889.02 | J/molxK | 1109.52 | Joback Method |
| dvisc | 0.0001063 | Paxs | 898.00 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0001277 | Paxs | 846.11 | Joback Method |
| dvisc | 0.0001570 | Paxs | 794.22 | Joback Method |
| dvisc | 0.0001988 | Paxs | 742.34 | Joback Method |
| dvisc | 0.0002607 | Paxs | 690.45 | Joback Method |
| dvisc | 0.0003573 | Paxs | 638.56 | Joback Method |
| dvisc | 0.0005178 | Paxs | 586.67 | 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=R530280&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|---------------------------------------|-------------------------------------------------|
| cp_g: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀w_s: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rin_{pol}: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/19-301-6/Glucose-3-methyl-acetylated.pdf>

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