# Sorbitol, 2,3,6-trimethyl, acetylated

**Inchi:** InChI=1S/C15H26O9/c1-9(16)22-8-12(20-5)14(21-6)15(24-11(3)18)13(7-19-4)23-10(2)17
**InchiKey:** ATVQUEJOBOKGCC-XGUBFFRZSA-N
**Formula:** C15H26O9
**SMILES:** COCC(OC(C)=O)C(OC(C)=O)C(OC)C(COC(C)=O)OC
**Mol. weight [g/mol]:** 350.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -951.10 | kJ/mol | Joback Method |
| hf | -1505.11 | kJ/mol | Joback Method |
| hfus | 32.44 | kJ/mol | Joback Method |
| hvap | 82.13 | kJ/mol | Joback Method |
| log10ws | -0.40 | | Crippen Method |
| logp | 0.089 | | Crippen Method |
| mcvol | 262.140 | ml/mol | McGowan Method |
| pc | 1551.22 | kPa | Joback Method |
| rinpol | 2251.00 | | NIST Webbook |
| rinpol | 2250.00 | | NIST Webbook |
| rinpol | 2251.00 | | NIST Webbook |
| tb | 836.97 | K | Joback Method |
| tc | 1032.72 | K | Joback Method |
| tf | 481.98 | K | Joback Method |
| vc | 0.978 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 815.80 | J/mol×K | 836.97 | Joback Method |
| cpg | 829.87 | J/mol×K | 869.59 | Joback Method |
| cpg | 842.71 | J/mol×K | 902.22 | Joback Method |
| cpg | 854.28 | J/mol×K | 934.84 | Joback Method |
| cpg | 864.53 | J/mol×K | 967.47 | Joback Method |
| cpg | 873.43 | J/mol×K | 1000.09 | Joback Method |
| cpg | 880.93 | J/mol×K | 1032.72 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004384 | Pa×s | 481.98 | Joback Method |
| dvisc | 0.0002053 | Pa×s | 541.14 | Joback Method |
| dvisc | 0.0001116 | Pa×s | 600.31 | Joback Method |
| dvisc | 0.0000677 | Pa×s | 659.48 | Joback Method |
| dvisc | 0.0000446 | Pa×s | 718.64 | Joback Method |
| dvisc | 0.0000313 | Pa×s | 777.81 | Joback Method |
| dvisc | 0.0000231 | Pa×s | 836.97 | 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=R527630&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 |