# Methyl 2,4,6-trihydroxybenzoate

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|---|---|
| **Other names:** | Methyl gallate |
| | Benzoic acid, 2,4,6-trihydroxy-, methyl ester |
| **Inchi:** | InChI=1S/C8H8O5/c1-13-8(12)7-5(10)2-4(9)3-6(7)11/h2-3,9-11H,1H3 |
| **InchiKey:** | AQDIJIAUYXOCGX-UHFFFAOYSA-N |
| **Formula:** | C8H8O5 |
| **SMILES:** | COC(=O)c1c(O)cc(O)cc1O |
| **Mol. weight [g/mol]:** | 184.15 |
| **CAS:** | 3147-39-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -568.89 | kJ/mol | Joback Method |
| hf | -748.65 | kJ/mol | Joback Method |
| hfus | 30.65 | kJ/mol | Joback Method |
| hvap | 83.88 | kJ/mol | Joback Method |
| log10ws | -0.36 | | Crippen Method |
| logp | 0.590 | | Crippen Method |
| mcvol | 124.870 | ml/mol | McGowan Method |
| pc | 7406.07 | kPa | Joback Method |
| tb | 727.27 | K | Joback Method |
| tc | 976.22 | K | Joback Method |
| tf | 613.66 | K | Joback Method |
| vc | 0.297 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 335.79 | J/mol×K | 727.27 | Joback Method |
| cpg | 343.51 | J/mol×K | 768.76 | Joback Method |
| cpg | 351.03 | J/mol×K | 810.25 | Joback Method |
| cpg | 358.55 | J/mol×K | 851.75 | Joback Method |
| cpg | 366.26 | J/mol×K | 893.24 | Joback Method |
| cpg | 374.35 | J/mol×K | 934.73 | Joback Method |
| cpg | 383.02 | J/mol×K | 976.22 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000014 | Pa×s | 613.66 | Joback Method |
| dvisc | 0.0000009 | Pa×s | 632.60 | Joback Method |
| dvisc | 0.0000006 | Pa×s | 651.53 | Joback Method |
| dvisc | 0.0000004 | Pa×s | 670.46 | Joback Method |
| dvisc | 0.0000003 | Pa×s | 689.40 | Joback Method |
| dvisc | 0.0000002 | Pa×s | 708.34 | Joback Method |
| dvisc | 0.0000001 | Pa×s | 727.27 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3147395&Units=SI |
| **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 |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |