# Benzenemehanol, 4-hydroxy-3-methoxy, acetate

**Inchi:** InChI=1S/C10H12O4/c1-7(11)14-6-8-3-4-9(12)10(5-8)13-2/h3-5,12H,6H2,1-2H3
**InchiKey:** DZWDEGBGKYCSKL-UHFFFAOYSA-N
**Formula:** C10H12O4
**SMILES:** COc1cc(COC(C)=O)ccc1O
**Mol. weight [g/mol]:** 196.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -357.44 | kJ/mol | Joback Method |
| hf | -579.00 | kJ/mol | Joback Method |
| hfus | 25.07 | kJ/mol | Joback Method |
| hvap | 65.37 | kJ/mol | Joback Method |
| log10ws | -1.72 | | Crippen Method |
| logp | 1.464 | | Crippen Method |
| mcvol | 147.180 | ml/mol | McGowan Method |
| pc | 3526.27 | kPa | Joback Method |
| tb | 639.19 | K | Joback Method |
| tc | 860.68 | K | Joback Method |
| tf | 447.51 | K | Joback Method |
| vc | 0.495 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 372.77 | J/mol×K | 639.19 | Joback Method |
| cpg | 384.49 | J/mol×K | 676.10 | Joback Method |
| cpg | 395.53 | J/mol×K | 713.02 | Joback Method |
| cpg | 405.91 | J/mol×K | 749.93 | Joback Method |
| cpg | 415.69 | J/mol×K | 786.85 | Joback Method |
| cpg | 424.90 | J/mol×K | 823.76 | Joback Method |
| cpg | 433.57 | J/mol×K | 860.68 | Joback Method |
| dvisc | 0.0003718 | Pa×s | 447.51 | Joback Method |
| dvisc | 0.0001978 | Pa×s | 479.46 | Joback Method |
| dvisc | 0.0001139 | Pa×s | 511.40 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000700 | Pa×s | 543.35 | Joback Method |
| dvisc | 0.0000454 | Pa×s | 575.30 | Joback Method |
| dvisc | 0.0000308 | Pa×s | 607.24 | Joback Method |
| dvisc | 0.0000217 | Pa×s | 639.19 | Joback Method |

# Sources

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|---|---|
| **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=R69952&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |

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