# Benzenepropanoic acid, 4-hydroxy-

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|---|---|
| **Other names:** | Phloretic acid |
| | Hydrocinnamic acid, p-hydroxy- |
| | «beta»-(p-Hydroxyphenyl)propionic acid |
| | p-Hydroxyhydrocinnamic acid |
| | p-Hydroxyphenylpropionic acid |
| | Hydro-p-coumaric acid |
| | 3-(p-Hydroxyphenyl)propionic acid |
| | 3-(4-Hydroxyphenyl)propanoic acid |
| | 3-(4-Hydroxyphenyl)propionic acid |
| | 4-Hydroxyphenylpropionic acid |
| | 3-(para-Hydroxyphenyl)-propionic acid |
| | Dihydro-p-coumaric acid |
| | 4-Hydroxybenzenepropanoic acid |
| | 3-(4'-Hydroxyphenyl)propionic acid |
| | 4-(2-Carboxyethyl)phenol |
| | NSC 40949 |
| **Inchi:** | InChI=1S/C9H10O3/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-2,4-5,10H,3,6H2,(H,11,12) |
| **InchiKey:** | NMHMNPHRMNGLLB-UHFFFAOYSA-N |
| **Formula:** | C9H10O3 |
| **SMILES:** | O=C(O)CCc1ccc(O)cc1 |
| **Mol. weight [g/mol]:** | 166.17 |
| **CAS:** | 501-97-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -283.05 | kJ/mol | Joback Method |
| hf | -434.68 | kJ/mol | Joback Method |
| hfus | 24.58 | kJ/mol | Joback Method |
| hvap | 74.34 | kJ/mol | Joback Method |
| log10ws | -1.34 | | Crippen Method |
| logp | 1.409 | | Crippen Method |
| mcvol | 127.220 | ml/mol | McGowan Method |
| pc | 4775.98 | kPa | Joback Method |
| rinpol | 1653.60 | | NIST Webbook |
| tb | 658.67 | K | Joback Method |
| tc | 871.60 | K | Joback Method |
| tf | 402.50 ± 0.50 | K | NIST Webbook |

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|---|---|---|---|
| vc | 0.422 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 325.04 | J/mol×K | 658.67 | Joback Method |
| cpg | 334.12 | J/mol×K | 694.16 | Joback Method |
| cpg | 342.62 | J/mol×K | 729.65 | Joback Method |
| cpg | 350.59 | J/mol×K | 765.14 | Joback Method |
| cpg | 358.12 | J/mol×K | 800.63 | Joback Method |
| cpg | 365.26 | J/mol×K | 836.12 | Joback Method |
| cpg | 372.09 | J/mol×K | 871.60 | Joback Method |
| dvisc | 0.0006700 | Pa×s | 440.08 | Joback Method |
| dvisc | 0.0002502 | Pa×s | 476.51 | Joback Method |
| dvisc | 0.0001075 | Pa×s | 512.94 | Joback Method |
| dvisc | 0.0000516 | Pa×s | 549.38 | Joback Method |
| dvisc | 0.0000272 | Pa×s | 585.81 | Joback Method |
| dvisc | 0.0000154 | Pa×s | 622.24 | Joback Method |
| dvisc | 0.0000093 | Pa×s | 658.67 | Joback Method |
| hfust | 28.90 | kJ/mol | 402.50 | NIST Webbook |

# 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=C501973&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

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|---|---|
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |