

2-Propenoic acid, 3-(4-hydroxyphenyl)-, (Z)-

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| Other names: | cis-p-coumaric acid cis-4-hydroxycinnamic acid |
| Inchi: | InChI=1S/C9H8O3/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-6,10H,(H,11,12)/b6-3- |
| InchiKey: | NGSWKAQJJWESNS-UTCJRWHESA-N |
| Formula: | C9H8O3 |
| SMILES: | O=C(O)C=Cc1ccc(O)cc1 |
| Mol. weight [g/mol]: | 164.16 |
| CAS: | 4501-31-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| chs | -4174.00 | kJ/mol | NIST Webbook |
| gf | -202.83 | kJ/mol | Joback Method |
| hf | -317.46 | kJ/mol | Joback Method |
| hfus | 24.78 | kJ/mol | Joback Method |
| hvap | 74.30 | kJ/mol | Joback Method |
| log10ws | -1.36 | | Crippen Method |
| logp | 1.490 | | Crippen Method |
| mcvol | 122.920 | ml/mol | McGowan Method |
| pc | 5138.68 | kPa | Joback Method |
| tb | 662.83 | K | Joback Method |
| tc | 884.22 | K | Joback Method |
| tf | 435.00 | K | Joback Method |
| vc | 0.403 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 302.19 | J/molxK | 662.83 | Joback Method |
| cpg | 310.51 | J/molxK | 699.73 | Joback Method |
| cpg | 318.25 | J/molxK | 736.63 | Joback Method |
| cpg | 325.49 | J/molxK | 773.52 | Joback Method |
| cpg | 332.34 | J/molxK | 810.42 | Joback Method |
| cpg | 338.88 | J/molxK | 847.32 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 345.20 | J/molxK | 884.22 | Joback Method |
| dvisc | 0.0006684 | Paxs | 435.00 | Joback Method |
| dvisc | 0.0002358 | Paxs | 472.97 | Joback Method |
| dvisc | 0.0000971 | Paxs | 510.94 | Joback Method |
| dvisc | 0.0000452 | Paxs | 548.91 | Joback Method |
| dvisc | 0.0000232 | Paxs | 586.89 | Joback Method |
| dvisc | 0.0000130 | Paxs | 624.86 | Joback Method |
| dvisc | 0.0000077 | Paxs | 662.83 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C4501319&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| chs: | Standard solid enthalpy of combustion |
| 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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