# P-HYDROXYBENZENESULFONIC ACID

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|---|---|
| **Other names:** | Benzenesulfonic acid, p-hydroxy- |
| | p-Hydroxybenzenesulfonic acid |
| | p-Phenolsulfonic acid |
| | p-Sulfophenol |
| | Hydroxybenzene-4-sulfonic acid |
| | 4-Hydroxybenzenesulfonic acid |
| | 4-Phenolsulfonic acid |
| | 4-Hydroxyphenylsulfonic acid |
| | p-Hydroxybenzenesulphonic acid |
| | NSC 227908 |
| | 4-hydroxybenzenesulphonic acid |
| **Inchi:** | InChI=1S/C6H6O4S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4,7H,(H,8,9,10) |
| **InchiKey:** | FEPBITJSIHRMRT-UHFFFAOYSA-N |
| **Formula:** | C6H6O4S |
| **SMILES:** | O=S(=O)(O)c1ccc(O)cc1 |
| **Mol. weight [g/mol]:** | 174.18 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -585.26 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 26.59 | kJ/mol | Joback Method |
| hvap | 119.43 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.31 | eV | Cheméo Relay (1.0) |
| log10ws | 0.01 | | Cheméo Relay (1.0) |
| logp | 0.639 | | Crippen Method |
| mcvol | 111.470 | ml/mol | McGowan Method |
| tb | 591.17 | K | Cheméo Relay (1.0) |
| tf | 527.96 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 255.58 | J/mol×K | 583.94 | Joback Method |
| cpg | 263.54 | J/mol×K | 618.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 270.90 | J/mol×K | 653.40 | Joback Method |
| cpg | 277.70 | J/mol×K | 688.13 | Joback Method |
| cpg | 283.99 | J/mol×K | 722.86 | Joback Method |
| cpg | 289.80 | J/mol×K | 757.59 | Joback Method |
| cpg | 295.19 | J/mol×K | 792.32 | Joback Method |

# Sources

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| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C98679&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |