

# Benzenesulfonic acid, 4-hydroxy-

**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]:** 174.17  
**CAS:** 98-67-9

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -647.93 | kJ/mol  | Joback Method  |
| hf            | -713.53 | kJ/mol  | Joback Method  |
| hfus          | 26.59   | kJ/mol  | Joback Method  |
| hvap          | 79.55   | kJ/mol  | Joback Method  |
| log10ws       | -0.61   |         | Crippen Method |
| logp          | 0.639   |         | Crippen Method |
| mcvol         | 111.470 | ml/mol  | McGowan Method |
| pc            | 8783.57 | kPa     | Joback Method  |
| tb            | 583.94  | K       | Joback Method  |
| tc            | 792.32  | K       | Joback Method  |
| tf            | 394.90  | K       | Joback Method  |
| vc            | 0.374   | m3/kmol | Joback Method  |

# 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 |
| 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

|                 |                                                                                                                                         |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C98679&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98679&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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