# Benzenesulfinic-acid-

**Other names:** benzenesulphinic acid
**Inchi:** InChI=1S/C6H6O2S/c7-9(8)6-4-2-1-3-5-6/h1-5H,(H,7,8)
**InchiKey:** JEHKKBHWRAXMCH-UHFFFAOYSA-N
**Formula:** C6H6O2S
**SMILES:** O=S(O)c1ccccc1
**Mol. weight [g/mol]:** 142.18
**CAS:** 618-41-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -242.48 | kJ/mol | Joback Method |
| hf | -288.61 | kJ/mol | Joback Method |
| hfus | 17.18 | kJ/mol | Joback Method |
| hvap | 60.63 | kJ/mol | Joback Method |
| log10ws | -0.86 | | Crippen Method |
| logp | 1.267 | | Crippen Method |
| mcvol | 99.730 | ml/mol | McGowan Method |
| pc | 6056.11 | kPa | Joback Method |
| tb | 513.82 | K | Joback Method |
| tc | 723.75 | K | Joback Method |
| tf | 281.10 | K | Joback Method |
| vc | 0.372 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 198.80 | J/mol×K | 513.82 | Joback Method |
| cpg | 207.70 | J/mol×K | 548.81 | Joback Method |
| cpg | 216.05 | J/mol×K | 583.80 | Joback Method |
| cpg | 223.85 | J/mol×K | 618.78 | Joback Method |
| cpg | 231.11 | J/mol×K | 653.77 | Joback Method |
| cpg | 237.85 | J/mol×K | 688.76 | Joback Method |
| cpg | 244.09 | J/mol×K | 723.75 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=C618417&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |