# O-AMINOBENZENESULFONIC ACID

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|---|---|
| **Other names:** | 1-Aminobenzene-2-sulfonic acid |
| | 2-Aminobenzenesulfonic acid |
| | 2-Aminobenzenesulphonic acid |
| | Aniline-2-sulfonic acid |
| | Aniline-o-sulphonic acid |
| | Anilino-2-sulfonic acid |
| | Anilino-o-sulfonic acid |
| | Anilino-o-sulphonic acid |
| | Benzenesulfonic acid, 2-amino- |
| | Benzenesulfonic acid, o-amino- |
| | NSC 147 |
| | Orthanilic acid |
| | o-Aminobenzenesulfonic acid |
| | o-Aminophenylsulfonic acid |
| | o-Sulfanilic acid |
| **Inchi:** | InChI=1S/C6H7NO3S/c7-5-3-1-2-4-6(5)11(8,9)10/h1-4H,7H2,(H,8,9,10) |
| **InchiKey:** | ZMCHBSMFKQYNKA-UHFFFAOYSA-N |
| **Formula:** | C6H7NO3S |
| **SMILES:** | Nc1ccccc1S(=O)(=O)O |
| **Mol. weight [g/mol]:** | 173.19 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3363.90 ± 0.60 | kJ/mol | NIST Webbook |
| hf | -437.37 | kJ/mol | Cheméo Relay (1.0) |
| hfs | -559.60 ± 1.10 | kJ/mol | NIST Webbook |
| hfus | 25.61 | kJ/mol | Joback Method |
| ie | 8.60 | eV | Cheméo Relay (1.0) |
| log10ws | -0.74 | | Cheméo Relay (1.0) |
| logp | 0.516 | | Crippen Method |
| mcvol | 115.580 | ml/mol | McGowan Method |
| tb | 598.58 | K | Cheméo Relay (1.0) |
| tf | 475.36 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 261.80 | J/mol×K | 580.83 | Joback Method |
| cpg | 270.63 | J/mol×K | 615.34 | Joback Method |
| cpg | 278.88 | J/mol×K | 649.86 | Joback Method |
| cpg | 286.56 | J/mol×K | 684.37 | Joback Method |
| cpg | 293.68 | J/mol×K | 718.89 | Joback Method |
| cpg | 300.24 | J/mol×K | 753.40 | Joback Method |
| cpg | 306.24 | J/mol×K | 787.92 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **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=C88211&Units=SI |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |