

# 4-Chloro-N-(2-hydroxypropionyl)-benzenesulfona

**Inchi:** InChI=1S/C9H10ClNO4S/c1-6(12)9(13)11-16(14,15)8-4-2-7(10)3-5-8/h2-6,12H,1H3,(H,1  
**InchiKey:** YHRUVVJCYRHQGX-UHFFFAOYSA-N  
**Formula:** C9H10ClNO4S  
**SMILES:** CC(O)C(O)=NS(=O)(=O)c1ccc(Cl)cc1  
**Mol. weight [g/mol]:** 263.70  
**CAS:** 90346-78-4

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -710.43 | kJ/mol | Joback Method  |
| hvap          | 97.95   | kJ/mol | Joback Method  |
| log10ws       | -2.04   |        | Crippen Method |
| logp          | 1.366   |        | Crippen Method |
| mcvol         | 171.660 | ml/mol | McGowan Method |
| pc            | 4130.29 | kPa    | Joback Method  |
| rinpol        | 2150.00 |        | NIST Webbook   |
| rinpol        | 2150.00 |        | NIST Webbook   |
| tb            | 782.67  | K      | Joback Method  |
| tc            | 986.94  | K      | Joback Method  |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C90346784&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**hf:** Enthalpy of formation at standard conditions

|                                       |   |
|---------------------------------------|---|
| <b>h<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log10 of Water solubility in mol/l              |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</b>              | McGowan's characteristic volume                 |
| <b>p<sub>c</sub>:</b>                 | Critical Pressure                               |
| <b>ri<sub>npol</sub>:</b>             | Non-polar retention indices                     |
| <b>t<sub>b</sub>:</b>                 | Normal Boiling Point Temperature                |
| <b>t<sub>c</sub>:</b>                 | Critical Temperature                            |

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