

# 1,3-Benzenediol, 4,6-dichloro-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Resorcinol, 4,6-dichloro-<br>4,6-Dichlororesorcinol<br>4,6-Dichloro-1,3-dihydroxybenzene<br>3,4-Dichlororesorcinol |
| <b>Inchi:</b>               | InChI=1S/C6H4Cl2O2/c7-3-1-4(8)6(10)2-5(3)9/h1-2,9-10H  |
| <b>InchiKey:</b>            | GRLQBYQELUWBIO-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C6H4Cl2O2  |
| <b>SMILES:</b>              | Oc1cc(O)c(Cl)cc1Cl   |
| <b>Mol. weight [g/mol]:</b> | 179.00   |
| <b>CAS:</b>                 | 137-19-9   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -230.68 | kJ/mol  | Joback Method  |
| hf            | -328.21 | kJ/mol  | Joback Method  |
| hfus          | 24.91   | kJ/mol  | Joback Method  |
| hvap          | 66.69   | kJ/mol  | Joback Method  |
| log10ws       | -1.94   |         | Crippen Method |
| logp          | 2.405   |         | Crippen Method |
| mcvol         | 107.860 | ml/mol  | McGowan Method |
| pc            | 6359.24 | kPa     | Joback Method  |
| tb            | 527.20  | K       | NIST Webbook   |
| tc            | 861.92  | K       | Joback Method  |
| tf            | 479.60  | K       | Joback Method  |
| vc            | 0.293   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 220.56 | J/molxK | 604.44          | Joback Method |
| cpg           | 226.43 | J/molxK | 647.35          | Joback Method |
| cpg           | 231.76 | J/molxK | 690.27          | Joback Method |
| cpg           | 236.70 | J/molxK | 733.18          | Joback Method |
| cpg           | 241.40 | J/molxK | 776.09          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 246.05    | J/mol×K | 819.00 | Joback Method |
| cpg   | 250.80    | J/mol×K | 861.92 | Joback Method |
| dvisc | 0.0001179 | Paxs    | 479.60 | Joback Method |
| dvisc | 0.0000687 | Paxs    | 500.41 | Joback Method |
| dvisc | 0.0000418 | Paxs    | 521.21 | Joback Method |
| dvisc | 0.0000264 | Paxs    | 542.02 | Joback Method |
| dvisc | 0.0000173 | Paxs    | 562.83 | Joback Method |
| dvisc | 0.0000117 | Paxs    | 583.63 | Joback Method |
| dvisc | 0.0000081 | Paxs    | 604.44 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C137199&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C137199&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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                                 |

Latest version available from:

<https://www.chemeo.com/cid/118-994-8/1-3-Benzenediol-4-6-dichloro.pdf>

Generated by Cheméo on 2024-04-26 07:07:06.666375667 +0000 UTC m=+16404475.586952988.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.