

# 3,5-Dichloro-4-hydroxybenzaldehyde

|                      |                                                                               |
|----------------------|-------------------------------------------------------------------------------|
| Other names:         | Benzaldehyde, 4-hydroxy-3,5-dichloro<br>Benzaldehyde, 3,5-dichloro-4-hydroxy- |
| Inchi:               | InChI=1S/C7H4Cl2O2/c8-5-1-4(3-10)2-6(9)7(5)11/h1-3,11H                        |
| InchiKey:            | LIYGCLJYTHRBQV-UHFFFAOYSA-N                                                   |
| Formula:             | C7H4Cl2O2                                                                     |
| SMILES:              | O=Cc1cc(Cl)c(O)c(Cl)c1                                                        |
| Mol. weight [g/mol]: | 191.01                                                                        |
| CAS:                 | 2314-36-5                                                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -176.79 | kJ/mol  | Joback Method  |
| hf            | -268.59 | kJ/mol  | Joback Method  |
| hfus          | 23.62   | kJ/mol  | Joback Method  |
| hvap          | 63.28   | kJ/mol  | Joback Method  |
| log10ws       | -2.63   |         | Crippen Method |
| logp          | 2.511   |         | Crippen Method |
| mcvol         | 117.650 | ml/mol  | McGowan Method |
| pc            | 4822.53 | kPa     | Joback Method  |
| rinpol        | 1465.00 |         | NIST Webbook   |
| rinpol        | 1476.00 |         | NIST Webbook   |
| rinpol        | 1479.00 |         | NIST Webbook   |
| rinpol        | 1463.00 |         | NIST Webbook   |
| rinpol        | 1457.00 |         | NIST Webbook   |
| rinpol        | 1465.00 |         | NIST Webbook   |
| rinpol        | 1465.00 |         | NIST Webbook   |
| rinpol        | 1465.00 |         | NIST Webbook   |
| rinpol        | 1467.00 |         | NIST Webbook   |
| tb            | 600.34  | K       | Joback Method  |
| tc            | 844.92  | K       | Joback Method  |
| tf            | 433.67  | K       | Joback Method  |
| vc            | 0.401   | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 234.27    | J/mol×K | 600.34          | Joback Method |
| cpg           | 263.28    | J/mol×K | 804.16          | Joback Method |
| cpg           | 258.26    | J/mol×K | 763.39          | Joback Method |
| cpg           | 252.93    | J/mol×K | 722.63          | Joback Method |
| cpg           | 247.21    | J/mol×K | 681.87          | Joback Method |
| cpg           | 241.01    | J/mol×K | 641.10          | Joback Method |
| cpg           | 268.07    | J/mol×K | 844.92          | Joback Method |
| dvisc         | 0.0000564 | Pa×s    | 600.34          | Joback Method |
| dvisc         | 0.0000776 | Pa×s    | 572.56          | Joback Method |
| dvisc         | 0.0001102 | Pa×s    | 544.78          | Joback Method |
| dvisc         | 0.0001627 | Pa×s    | 517.00          | Joback Method |
| dvisc         | 0.0002511 | Pa×s    | 489.23          | Joback Method |
| dvisc         | 0.0004081 | Pa×s    | 461.45          | Joback Method |
| dvisc         | 0.0007061 | Pa×s    | 433.67          | Joback Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                           |
| 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=C2314365&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2314365&amp;Units=SI</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>rinpol:</b> | Non-polar retention indices      |
| <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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