

# 3,4-Dichlorobenzyl alcohol

|                      |                                                                 |
|----------------------|-----------------------------------------------------------------|
| Other names:         | Benzenemethanol, 3,4-dichloro-<br>Benzyl alcohol, 3,4-dichloro- |
| Inchi:               | InChI=1S/C7H6Cl2O/c8-6-2-1-5(4-10)3-7(6)9/h1-3,10H,4H2          |
| InchiKey:            | FVJIUQSKXOYFKG-UHFFFAOYSA-N                                     |
| Formula:             | C7H6Cl2O                                                        |
| SMILES:              | OCc1ccc(Cl)c(Cl)c1                                              |
| Mol. weight [g/mol]: | 177.03                                                          |
| CAS:                 | 1805-32-9                                                       |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -59.47  | kJ/mol  | Joback Method  |
| hf            | -157.93 | kJ/mol  | Joback Method  |
| hfus          | 19.63   | kJ/mol  | Joback Method  |
| hvap          | 60.22   | kJ/mol  | Joback Method  |
| log10ws       | -2.98   |         | Crippen Method |
| logp          | 2.486   |         | Crippen Method |
| mcvol         | 116.080 | ml/mol  | McGowan Method |
| pc            | 4051.80 | kPa     | Joback Method  |
| tb            | 563.24  | K       | Joback Method  |
| tc            | 775.59  | K       | Joback Method  |
| tf            | 340.77  | K       | Joback Method  |
| vc            | 0.436   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 224.64 | J/mol×K | 563.24          | Joback Method |
| cpg           | 258.50 | J/mol×K | 740.20          | Joback Method |
| cpg           | 252.60 | J/mol×K | 704.81          | Joback Method |
| cpg           | 246.28 | J/mol×K | 669.42          | Joback Method |
| cpg           | 239.53 | J/mol×K | 634.02          | Joback Method |
| cpg           | 232.32 | J/mol×K | 598.63          | Joback Method |
| cpg           | 264.01 | J/mol×K | 775.59          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001210 | Pa×s | 563.24 | Joback Method |
| dvisc | 0.0001753 | Pa×s | 526.16 | Joback Method |
| dvisc | 0.0002687 | Pa×s | 489.08 | Joback Method |
| dvisc | 0.0004416 | Pa×s | 452.00 | Joback Method |
| dvisc | 0.0007932 | Pa×s | 414.93 | Joback Method |
| dvisc | 0.0015984 | Pa×s | 377.85 | Joback Method |
| dvisc | 0.0037516 | Pa×s | 340.77 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1805329&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1805329&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>                                       |

## 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                                 |

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