

# 2,3-Dichlorobenzyl alcohol, 1-methylpropyl ether

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C11H14Cl2O/c1-3-8(2)14-7-9-5-4-6-10(12)11(9)13/h4-6,8H,3,7H2,1-2H3 |
| InchiKey:            | NLSURMQCIQWYBX-UHFFFAOYSA-N   |
| Formula:             | C11H14Cl2O  |
| SMILES:              | CCC(C)OCc1cccc(Cl)c1Cl  |
| Mol. weight [g/mol]: | 233.13  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 3.59    | kJ/mol               | Joback Method  |
| hf            | -225.76 | kJ/mol               | Joback Method  |
| hfus          | 23.57   | kJ/mol               | Joback Method  |
| hvap          | 54.47   | kJ/mol               | Joback Method  |
| log10ws       | -4.59   |                      | Crippen Method |
| logp          | 4.308   |                      | Crippen Method |
| mvol          | 172.440 | ml/mol               | McGowan Method |
| pc            | 2365.67 | kPa                  | Joback Method  |
| rinpol        | 1584.00 |                      | NIST Webbook   |
| rinpol        | 1584.00 |                      | NIST Webbook   |
| tb            | 584.56  | K                    | Joback Method  |
| tc            | 800.88  | K                    | Joback Method  |
| tf            | 332.26  | K                    | Joback Method  |
| vc            | 0.653   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 382.37    | J/molxK | 584.56          | Joback Method |
| cpg           | 396.17    | J/molxK | 620.61          | Joback Method |
| cpg           | 409.20    | J/molxK | 656.67          | Joback Method |
| cpg           | 421.48    | J/molxK | 692.72          | Joback Method |
| cpg           | 433.01    | J/molxK | 728.77          | Joback Method |
| cpg           | 443.83    | J/molxK | 764.82          | Joback Method |
| cpg           | 453.94    | J/molxK | 800.88          | Joback Method |
| dvisc         | 0.0016170 | Paxs    | 332.26          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008859 | Paxs | 374.31 | Joback Method |
| dvisc | 0.0005481 | Paxs | 416.36 | Joback Method |
| dvisc | 0.0003703 | Paxs | 458.41 | Joback Method |
| dvisc | 0.0002672 | Paxs | 500.46 | Joback Method |
| dvisc | 0.0002029 | Paxs | 542.51 | Joback Method |
| dvisc | 0.0001602 | Paxs | 584.56 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375306&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375306&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>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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