

2,4-Dichlorobenzyl alcohol, 3-methylbutyl ether

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|----------------------|---|
| Inchi: | InChI=1S/C12H16Cl2O/c1-9(2)5-6-15-8-10-3-4-11(13)7-12(10)14/h3-4,7,9H,5-6,8H2,1-2 |
| InchiKey: | RNEBDJXOJVRGBF-UHFFFAOYSA-N |
| Formula: | C12H16Cl2O |
| SMILES: | CC(C)CCOCc1ccc(Cl)cc1Cl |
| Mol. weight [g/mol]: | 247.16 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 12.01 | kJ/mol | Joback Method |
| hf | -246.40 | kJ/mol | Joback Method |
| hfus | 26.16 | kJ/mol | Joback Method |
| hvap | 56.70 | kJ/mol | Joback Method |
| log10ws | -4.66 | | Crippen Method |
| logp | 4.556 | | Crippen Method |
| mcvol | 186.530 | ml/mol | McGowan Method |
| pc | 2159.31 | kPa | Joback Method |
| rinsol | 1667.00 | | NIST Webbook |
| tb | 607.44 | K | Joback Method |
| tc | 820.11 | K | Joback Method |
| tf | 343.53 | K | Joback Method |
| vc | 0.710 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 430.61 | J/molxK | 607.44 | Joback Method |
| cpg | 445.15 | J/molxK | 642.88 | Joback Method |
| cpg | 458.88 | J/molxK | 678.33 | Joback Method |
| cpg | 471.81 | J/molxK | 713.77 | Joback Method |
| cpg | 483.97 | J/molxK | 749.22 | Joback Method |
| cpg | 495.37 | J/molxK | 784.66 | Joback Method |
| cpg | 506.02 | J/molxK | 820.11 | Joback Method |
| dvisc | 0.0015502 | Paxs | 343.53 | Joback Method |
| dvisc | 0.0008347 | Paxs | 387.51 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005098 | Paxs | 431.50 | Joback Method |
| dvisc | 0.0003412 | Paxs | 475.49 | Joback Method |
| dvisc | 0.0002444 | Paxs | 519.47 | Joback Method |
| dvisc | 0.0001844 | Paxs | 563.46 | Joback Method |
| dvisc | 0.0001449 | Paxs | 607.44 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U378109&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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