

2,5-Dichlorobenzyl alcohol, n-pentyl ether

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H16Cl2O/c1-2-3-4-7-15-9-10-8-11(13)5-6-12(10)14/h5-6,8H,2-4,7,9H2,1H3 |
| InchiKey: | SHFXRECICDCIE-UHFFFAOYSA-N |
| Formula: | C12H16Cl2O |
| SMILES: | CCCCCOCc1cc(Cl)ccc1Cl |
| Mol. weight [g/mol]: | 247.16 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 14.45 | kJ/mol | Joback Method |
| hf | -241.12 | kJ/mol | Joback Method |
| hfus | 29.68 | kJ/mol | Joback Method |
| hvap | 57.09 | kJ/mol | Joback Method |
| log10ws | -4.90 | | Crippen Method |
| logp | 4.700 | | Crippen Method |
| mvol | 186.530 | ml/mol | McGowan Method |
| pc | 2143.35 | kPa | Joback Method |
| rinpol | 1704.00 | | NIST Webbook |
| tb | 607.88 | K | Joback Method |
| tc | 816.32 | K | Joback Method |
| tf | 358.53 | K | Joback Method |
| vc | 0.716 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 430.18 | J/molxK | 607.88 | Joback Method |
| cpg | 493.65 | J/molxK | 781.58 | Joback Method |
| cpg | 482.43 | J/molxK | 746.84 | Joback Method |
| cpg | 470.49 | J/molxK | 712.10 | Joback Method |
| cpg | 457.81 | J/molxK | 677.36 | Joback Method |
| cpg | 444.38 | J/molxK | 642.62 | Joback Method |
| cpg | 504.17 | J/molxK | 816.32 | Joback Method |
| dvisc | 0.0001554 | Paxs | 607.88 | Joback Method |
| dvisc | 0.0001939 | Paxs | 566.32 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002507 | Paxs | 524.76 | Joback Method |
| dvisc | 0.0003387 | Paxs | 483.20 | Joback Method |
| dvisc | 0.0004843 | Paxs | 441.65 | Joback Method |
| dvisc | 0.0007459 | Paxs | 400.09 | Joback Method |
| dvisc | 0.0012696 | Paxs | 358.53 | 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=U378123&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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<https://www.chemeo.com/cid/29-031-5/2-5-Dichlorobenzyl-alcohol-n-pentyl-ether.pdf>

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