

3,5-Dichlorobenzyl alcohol, n-butyl ether

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|-----------------------------|---|
| Inchi: | InChI=1S/C11H14Cl2O/c1-2-3-4-14-8-9-5-10(12)7-11(13)6-9/h5-7H,2-4,8H2,1H3 |
| InchiKey: | FUKPRAUYLWLWEE-UHFFFAOYSA-N |
| Formula: | C11H14Cl2O |
| SMILES: | CCCCOCc1cc(Cl)cc(Cl)c1 |
| Mol. weight [g/mol]: | 233.13 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 6.03 | kJ/mol | Joback Method |
| hf | -220.48 | kJ/mol | Joback Method |
| hfus | 27.09 | kJ/mol | Joback Method |
| hvap | 54.86 | kJ/mol | Joback Method |
| log10ws | -4.48 | | Crippen Method |
| logp | 4.310 | | Crippen Method |
| mcvol | 172.440 | ml/mol | McGowan Method |
| pc | 2347.36 | kPa | Joback Method |
| rinpol | 1606.00 | | NIST Webbook |
| rinpol | 1606.00 | | NIST Webbook |
| tb | 585.00 | K | Joback Method |
| tc | 796.84 | K | Joback Method |
| tf | 347.26 | K | Joback Method |
| vc | 0.659 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 381.96 | J/molxK | 585.00 | Joback Method |
| cpg | 395.42 | J/molxK | 620.31 | Joback Method |
| cpg | 408.15 | J/molxK | 655.61 | Joback Method |
| cpg | 420.17 | J/molxK | 690.92 | Joback Method |
| cpg | 431.48 | J/molxK | 726.23 | Joback Method |
| cpg | 442.12 | J/molxK | 761.53 | Joback Method |
| cpg | 452.09 | J/molxK | 796.84 | Joback Method |
| dvisc | 0.0013156 | Paxs | 347.26 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0007871 | Paxs | 386.88 | Joback Method |
| dvisc | 0.0005181 | Paxs | 426.51 | Joback Method |
| dvisc | 0.0003661 | Paxs | 466.13 | Joback Method |
| dvisc | 0.0002732 | Paxs | 505.75 | Joback Method |
| dvisc | 0.0002127 | Paxs | 545.38 | Joback Method |
| dvisc | 0.0001713 | Paxs | 585.00 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U378139&Units=SI |
| 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 |

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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