

# 2,5-Dichlorobenzyl alcohol, tert.-butyl ether

|                      |                                                                         |
|----------------------|-------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C11H14Cl2O/c1-11(2,3)14-7-8-6-9(12)4-5-10(8)13/h4-6H,7H2,1-3H3 |
| InchiKey:            | HHRQHIPLNPOIOL-UHFFFAOYSA-N                                             |
| Formula:             | C11H14Cl2O                                                              |
| SMILES:              | CC(C)(C)OCc1cc(Cl)ccc1Cl                                                |
| Mol. weight [g/mol]: | 233.13                                                                  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 8.87    | kJ/mol  | Joback Method  |
| hf            | -229.23 | kJ/mol  | Joback Method  |
| hfus          | 19.68   | kJ/mol  | Joback Method  |
| hvap          | 53.56   | kJ/mol  | Joback Method  |
| log10ws       | -4.59   |         | Crippen Method |
| logp          | 4.308   |         | Crippen Method |
| mcvol         | 172.440 | ml/mol  | McGowan Method |
| pc            | 2391.19 | kPa     | Joback Method  |
| rinpol        | 1505.00 |         | NIST Webbook   |
| rinpol        | 1505.00 |         | NIST Webbook   |
| tb            | 581.77  | K       | Joback Method  |
| tc            | 806.74  | K       | Joback Method  |
| tf            | 349.68  | K       | Joback Method  |
| vc            | 0.648   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 385.44    | J/mol×K | 581.77          | Joback Method |
| cpg           | 447.75    | J/mol×K | 769.24          | Joback Method |
| cpg           | 436.98    | J/mol×K | 731.75          | Joback Method |
| cpg           | 425.41    | J/mol×K | 694.25          | Joback Method |
| cpg           | 412.99    | J/mol×K | 656.76          | Joback Method |
| cpg           | 399.68    | J/mol×K | 619.26          | Joback Method |
| cpg           | 457.75    | J/mol×K | 806.74          | Joback Method |
| dvisc         | 0.0001544 | Pa×s    | 581.77          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001968 | Pa×s | 543.09 | Joback Method |
| dvisc | 0.0002604 | Pa×s | 504.41 | Joback Method |
| dvisc | 0.0003609 | Pa×s | 465.73 | Joback Method |
| dvisc | 0.0005307 | Pa×s | 427.04 | Joback Method |
| dvisc | 0.0008427 | Pa×s | 388.36 | Joback Method |
| dvisc | 0.0014821 | Pa×s | 349.68 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U378122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U378122&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>                         |

## 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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