# 2,4-dichlorobenzyl pentadecyl ether

**Inchi:** InChI=1S/C22H36Cl2O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-25-19-20-15-16-21(23)18-
**InchiKey:** DQOSXTYICPYLDO-UHFFFAOYSA-N
**Formula:** C22H36Cl2O
**SMILES:** CCCCCCCCCCCCCCCOCc1ccc(Cl)cc1Cl
**Mol. weight [g/mol]:** 387.43

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 98.65 | kJ/mol | Joback Method |
| hf | -447.52 | kJ/mol | Joback Method |
| hfus | 55.58 | kJ/mol | Joback Method |
| hvap | 79.35 | kJ/mol | Joback Method |
| log10ws | -9.09 | | Crippen Method |
| logp | 8.601 | | Crippen Method |
| mcvol | 327.430 | ml/mol | McGowan Method |
| pc | 1027.28 | kPa | Joback Method |
| rinpol | 2693.00 | | NIST Webbook |
| rinpol | 2702.00 | | NIST Webbook |
| rinpol | 2693.00 | | NIST Webbook |
| rinpol | 2699.00 | | NIST Webbook |
| rinpol | 2702.00 | | NIST Webbook |
| rinpol | 2705.00 | | NIST Webbook |
| rinpol | 2696.00 | | NIST Webbook |
| rinpol | 2704.00 | | NIST Webbook |
| rinpol | 2705.00 | | NIST Webbook |
| rinpol | 2693.00 | | NIST Webbook |
| rinpol | 2699.00 | | NIST Webbook |
| rinpol | 2705.00 | | NIST Webbook |
| rinpol | 2706.00 | | NIST Webbook |
| rinpol | 2695.00 | | NIST Webbook |
| rinpol | 2698.00 | | NIST Webbook |
| tb | 836.68 | K | Joback Method |
| tc | 1032.34 | K | Joback Method |
| tf | 471.23 | K | Joback Method |
| vc | 1.276 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 984.66 | J/mol×K | 836.68 | Joback Method |
| cpg | 1002.73 | J/mol×K | 869.29 | Joback Method |
| cpg | 1019.72 | J/mol×K | 901.90 | Joback Method |
| cpg | 1035.68 | J/mol×K | 934.51 | Joback Method |
| cpg | 1050.65 | J/mol×K | 967.12 | Joback Method |
| cpg | 1064.65 | J/mol×K | 999.73 | Joback Method |
| cpg | 1077.74 | J/mol×K | 1032.34 | Joback Method |
| dvisc | 0.0005896 | Pa×s | 471.23 | Joback Method |
| dvisc | 0.0003003 | Pa×s | 532.14 | Joback Method |
| dvisc | 0.0001757 | Pa×s | 593.05 | Joback Method |
| dvisc | 0.0001136 | Pa×s | 653.95 | Joback Method |
| dvisc | 0.0000791 | Pa×s | 714.86 | Joback Method |
| dvisc | 0.0000583 | Pa×s | 775.77 | Joback Method |
| dvisc | 0.0000449 | Pa×s | 836.68 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R32339&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**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 |