# Diglycolic acid, 4-chlorobenzyl isobutyl ester

**Inchi:** InChI=1S/C15H19ClO5/c1-11(2)7-20-14(17)9-19-10-15(18)21-8-12-3-5-13(16)6-4-12/h3-
**InchiKey:** GNXNJKXFDAZWEX-UHFFFAOYSA-N
**Formula:** C15H19ClO5
**SMILES:** CC(C)COC(=O)COCC(=O)OCc1ccc(Cl)cc1
**Mol. weight [g/mol]:** 314.76

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -409.01 | kJ/mol | Joback Method |
| hf | -770.71 | kJ/mol | Joback Method |
| hfus | 35.69 | kJ/mol | Joback Method |
| hvap | 76.64 | kJ/mol | Joback Method |
| log10ws | -2.96 | | Crippen Method |
| logp | 2.599 | | Crippen Method |
| mcvol | 231.440 | ml/mol | McGowan Method |
| pc | 1896.95 | kPa | Joback Method |
| rinpol | 2779.00 | | NIST Webbook |
| rinpol | 2779.00 | | NIST Webbook |
| tb | 786.25 | K | Joback Method |
| tc | 995.37 | K | Joback Method |
| tf | 479.22 | K | Joback Method |
| vc | 0.876 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 647.42 | J/mol×K | 786.25 | Joback Method |
| cpg | 660.93 | J/mol×K | 821.10 | Joback Method |
| cpg | 673.40 | J/mol×K | 855.96 | Joback Method |
| cpg | 684.84 | J/mol×K | 890.81 | Joback Method |
| cpg | 695.24 | J/mol×K | 925.66 | Joback Method |
| cpg | 704.61 | J/mol×K | 960.51 | Joback Method |
| cpg | 712.94 | J/mol×K | 995.37 | Joback Method |
| dvisc | 0.0006317 | Pa×s | 479.22 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0003615 | Pa×s | 530.39 | Joback Method |
| dvisc | 0.0002282 | Pa×s | 581.56 | Joback Method |
| dvisc | 0.0001552 | Pa×s | 632.74 | Joback Method |
| dvisc | 0.0001118 | Pa×s | 683.91 | Joback Method |
| dvisc | 0.0000843 | Pa×s | 735.08 | Joback Method |
| dvisc | 0.0000660 | Pa×s | 786.25 | Joback Method |

# Sources

| | |
|---|---|
| **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=U382255&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |