# Diglycolic acid, butyl 2,6-dichlorophenyl ester

**Inchi:** InChI=1S/C14H16Cl2O5/c1-2-3-7-20-12(17)8-19-9-13(18)21-14-10(15)5-4-6-11(14)16/h4
**InchiKey:** VWAJLZMERUXVOJ-UHFFFAOYSA-N
**Formula:** C14H16Cl2O5
**SMILES:** CCCCOC(=O)COCC(=O)Oc1c(Cl)cccc1Cl
**Mol. weight [g/mol]:** 335.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -436.55 | kJ/mol | Joback Method |
| hf | -772.00 | kJ/mol | Joback Method |
| hfus | 40.43 | kJ/mol | Joback Method |
| hvap | 79.85 | kJ/mol | Joback Method |
| log10ws | -3.62 | | Crippen Method |
| logp | 3.259 | | Crippen Method |
| mcvol | 229.590 | ml/mol | McGowan Method |
| pc | 1957.87 | kPa | Joback Method |
| rinpol | 2730.00 | | NIST Webbook |
| rinpol | 2730.00 | | NIST Webbook |
| tb | 806.22 | K | Joback Method |
| tc | 1018.57 | K | Joback Method |
| tf | 525.39 | K | Joback Method |
| vc | 0.875 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 614.67 | J/mol×K | 806.22 | Joback Method |
| cpg | 626.44 | J/mol×K | 841.61 | Joback Method |
| cpg | 637.25 | J/mol×K | 877.00 | Joback Method |
| cpg | 647.07 | J/mol×K | 912.39 | Joback Method |
| cpg | 655.89 | J/mol×K | 947.78 | Joback Method |
| cpg | 663.71 | J/mol×K | 983.17 | Joback Method |
| cpg | 670.52 | J/mol×K | 1018.57 | Joback Method |
| dvisc | 0.0004517 | Pa×s | 525.39 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002939 | Pa×s | 572.19 | Joback Method |
| dvisc | 0.0002041 | Pa×s | 619.00 | Joback Method |
| dvisc | 0.0001491 | Pa×s | 665.81 | Joback Method |
| dvisc | 0.0001136 | Pa×s | 712.61 | Joback Method |
| dvisc | 0.0000895 | Pa×s | 759.41 | Joback Method |
| dvisc | 0.0000724 | Pa×s | 806.22 | Joback Method |

# Sources

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|---|---|
| **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=U382298&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 |