# Diglycolic acid, 4-chloro-2-methylphenyl hexyl ester

**Inchi:** InChI=1S/C17H23ClO5/c1-3-4-5-6-9-22-16(19)11-21-12-17(20)23-15-8-7-14(18)10-13(15
**InchiKey:** DRQYRDFZIXIMAH-UHFFFAOYSA-N
**Formula:** C17H23ClO5
**SMILES:** CCCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1C
**Mol. weight [g/mol]:** 342.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -399.36 | kJ/mol | Joback Method |
| hf | -818.18 | kJ/mol | Joback Method |
| hfus | 44.01 | kJ/mol | Joback Method |
| hvap | 82.14 | kJ/mol | Joback Method |
| log10ws | -4.24 | | Crippen Method |
| logp | 3.694 | | Crippen Method |
| mcvol | 259.620 | ml/mol | McGowan Method |
| pc | 1586.01 | kPa | Joback Method |
| rinpol | 2956.00 | | NIST Webbook |
| rinpol | 2956.00 | | NIST Webbook |
| tb | 837.43 | K | Joback Method |
| tc | 1042.91 | K | Joback Method |
| tf | 529.28 | K | Joback Method |
| vc | 0.995 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 758.01 | J/mol×K | 837.43 | Joback Method |
| cpg | 771.77 | J/mol×K | 871.68 | Joback Method |
| cpg | 784.43 | J/mol×K | 905.92 | Joback Method |
| cpg | 796.00 | J/mol×K | 940.17 | Joback Method |
| cpg | 806.47 | J/mol×K | 974.41 | Joback Method |
| cpg | 815.84 | J/mol×K | 1008.66 | Joback Method |
| cpg | 824.12 | J/mol×K | 1042.91 | Joback Method |
| dvisc | 0.0004050 | Pa×s | 529.28 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002506 | Pa×s | 580.64 | Joback Method |
| dvisc | 0.0001677 | Pa×s | 632.00 | Joback Method |
| dvisc | 0.0001192 | Pa×s | 683.36 | Joback Method |
| dvisc | 0.0000888 | Pa×s | 734.71 | Joback Method |
| dvisc | 0.0000688 | Pa×s | 786.07 | Joback Method |
| dvisc | 0.0000550 | Pa×s | 837.43 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382743&Units=SI |

# 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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