# Glutaric acid, 2-chloro-5-methylphenyl pentyl ester

**Inchi:** InChI=1S/C17H23ClO4/c1-3-4-5-11-21-16(19)7-6-8-17(20)22-15-12-13(2)9-10-14(15)18/

**InchiKey:** AKVKXVHUODQQQY-UHFFFAOYSA-N

**Formula:** C17H23ClO4

**SMILES:** CCCCCOC(=O)CCCC(=O)Oc1cc(C)ccc1Cl

**Mol. weight [g/mol]:** 326.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -294.36 | kJ/mol | Joback Method |
| hf | -685.96 | kJ/mol | Joback Method |
| hfus | 42.82 | kJ/mol | Joback Method |
| hvap | 79.73 | kJ/mol | Joback Method |
| log10ws | -5.16 | | Crippen Method |
| logp | 4.458 | | Crippen Method |
| mcvol | 253.750 | ml/mol | McGowan Method |
| pc | 1607.71 | kPa | Joback Method |
| rinpol | 2373.00 | | NIST Webbook |
| rinpol | 2373.00 | | NIST Webbook |
| tb | 815.01 | K | Joback Method |
| tc | 1020.37 | K | Joback Method |
| tf | 507.05 | K | Joback Method |
| vc | 0.977 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 730.36 | J/mol×K | 815.01 | Joback Method |
| cpg | 744.56 | J/mol×K | 849.24 | Joback Method |
| cpg | 757.73 | J/mol×K | 883.46 | Joback Method |
| cpg | 769.90 | J/mol×K | 917.69 | Joback Method |
| cpg | 781.06 | J/mol×K | 951.91 | Joback Method |
| cpg | 791.23 | J/mol×K | 986.14 | Joback Method |
| cpg | 800.43 | J/mol×K | 1020.37 | Joback Method |
| dvisc | 0.0005664 | Pa×s | 507.05 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003441 | Pa×s | 558.38 | Joback Method |
| dvisc | 0.0002273 | Pa×s | 609.70 | Joback Method |
| dvisc | 0.0001601 | Pa×s | 661.03 | Joback Method |
| dvisc | 0.0001187 | Pa×s | 712.36 | Joback Method |
| dvisc | 0.0000915 | Pa×s | 763.68 | Joback Method |
| dvisc | 0.0000730 | Pa×s | 815.01 | Joback Method |

# Sources

| | |
|---|---|
| **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=U359333&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |