# Glutaric acid, 2-chloro-6-fluorophenyl hexyl ester

**Inchi:** InChI=1S/C17H22ClFO4/c1-2-3-4-5-12-22-15(20)10-7-11-16(21)23-17-13(18)8-6-9-14(1
**InchiKey:** YDRRKXAGOQPLMQ-UHFFFAOYSA-N
**Formula:** C17H22ClFO4
**SMILES:** CCCCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
**Mol. weight [g/mol]:** 344.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -489.17 | kJ/mol | Joback Method |
| hf | -882.07 | kJ/mol | Joback Method |
| hfus | 45.90 | kJ/mol | Joback Method |
| hvap | 78.92 | kJ/mol | Joback Method |
| log10ws | -5.43 | | Crippen Method |
| logp | 4.678 | | Crippen Method |
| mcvol | 255.520 | ml/mol | McGowan Method |
| pc | 1551.22 | kPa | Joback Method |
| rinpol | 2301.00 | | NIST Webbook |
| rinpol | 2301.00 | | NIST Webbook |
| tb | 814.28 | K | Joback Method |
| tc | 1014.35 | K | Joback Method |
| tf | 507.64 | K | Joback Method |
| vc | 0.995 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 737.88 | J/mol×K | 814.28 | Joback Method |
| cpg | 751.62 | J/mol×K | 847.62 | Joback Method |
| cpg | 764.38 | J/mol×K | 880.97 | Joback Method |
| cpg | 776.17 | J/mol×K | 914.31 | Joback Method |
| cpg | 787.02 | J/mol×K | 947.66 | Joback Method |
| cpg | 796.92 | J/mol×K | 981.00 | Joback Method |
| cpg | 805.90 | J/mol×K | 1014.35 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391514&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

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |