# Glutaric acid, 1-cyclopentylethyl 2-chloro-6-fluorophenyl ester

**Inchi:** InChI=1S/C18H22ClFO4/c1-12(13-6-2-3-7-13)23-16(21)10-5-11-17(22)24-18-14(19)8-4-9

**InchiKey:** JKQYUFSIGJLUES-UHFFFAOYSA-N

**Formula:** C18H22ClFO4

**SMILES:** CC(OC(=O)CCCC(=O)Oc1c(F)cccc1Cl)C1CCCC1

**Mol. weight [g/mol]:** 356.82

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -446.64 | kJ/mol | Joback Method |
| hf | -847.51 | kJ/mol | Joback Method |
| hfus | 38.90 | kJ/mol | Joback Method |
| hvap | 81.01 | kJ/mol | Joback Method |
| log10ws | -5.62 | | Crippen Method |
| logp | 4.677 | | Crippen Method |
| mcvol | 258.750 | ml/mol | McGowan Method |
| pc | 1670.06 | kPa | Joback Method |
| rinpol | 2381.00 | | NIST Webbook |
| rinpol | 2381.00 | | NIST Webbook |
| tb | 852.00 | K | Joback Method |
| tc | 1070.41 | K | Joback Method |
| tf | 514.81 | K | Joback Method |
| vc | 0.986 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 785.63 | J/mol×K | 852.00 | Joback Method |
| cpg | 800.33 | J/mol×K | 888.40 | Joback Method |
| cpg | 813.76 | J/mol×K | 924.80 | Joback Method |
| cpg | 825.93 | J/mol×K | 961.21 | Joback Method |
| cpg | 836.89 | J/mol×K | 997.61 | Joback Method |
| cpg | 846.67 | J/mol×K | 1034.01 | Joback Method |
| cpg | 855.29 | J/mol×K | 1070.41 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405465&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 |