# Glutaric acid, hex-4-en-1-yl 2-chloro-6-fluorophenyl ester

**Inchi:** InChI=1S/C17H20ClFO4/c1-2-3-4-5-12-22-15(20)10-7-11-16(21)23-17-13(18)8-6-9-14(1
**InchiKey:** ZEASSUCKBVMGTA-NSCUHMNNSA-N
**Formula:** C17H20ClFO4
**SMILES:** CC=CCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
**Mol. weight [g/mol]:** 342.79

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -408.95 | kJ/mol | Joback Method |
| hf | -764.85 | kJ/mol | Joback Method |
| hfus | 46.10 | kJ/mol | Joback Method |
| hvap | 78.87 | kJ/mol | Joback Method |
| log10ws | -5.29 | | Crippen Method |
| logp | 4.454 | | Crippen Method |
| mcvol | 251.220 | ml/mol | McGowan Method |
| pc | 1616.77 | kPa | Joback Method |
| rinpol | 2298.00 | | NIST Webbook |
| rinpol | 2298.00 | | NIST Webbook |
| tb | 818.44 | K | Joback Method |
| tc | 1023.34 | K | Joback Method |
| tf | 502.56 | K | Joback Method |
| vc | 0.975 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 711.69 | J/mol×K | 818.44 | Joback Method |
| cpg | 724.91 | J/mol×K | 852.59 | Joback Method |
| cpg | 737.20 | J/mol×K | 886.74 | Joback Method |
| cpg | 748.57 | J/mol×K | 920.89 | Joback Method |
| cpg | 759.06 | J/mol×K | 955.04 | Joback Method |
| cpg | 768.69 | J/mol×K | 989.19 | Joback Method |
| cpg | 777.48 | J/mol×K | 1023.34 | Joback Method |

# Sources

| | |
|---|---|
| **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=U405304&Units=SI |

# Legend

| | |
|---|---|
| **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 |