# Glutaric acid, di(1-(2-fluorophenyl)ethyl) ester

**Inchi:** InChI=1S/C21H22F2O4/c1-14(16-8-3-5-10-18(16)22)26-20(24)12-7-13-21(25)27-15(2)17
**InchiKey:** YAMDPLKCGDGOTG-UHFFFAOYSA-N
**Formula:** C21H22F2O4
**SMILES:** CC(OC(=O)CCCC(=O)OC(C)c1ccccc1F)c1ccccc1F
**Mol. weight [g/mol]:** 376.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -530.84 | kJ/mol | Joback Method |
| hf | -919.03 | kJ/mol | Joback Method |
| hfus | 42.14 | kJ/mol | Joback Method |
| hvap | 84.12 | kJ/mol | Joback Method |
| log10ws | -6.12 | | Crippen Method |
| logp | 5.044 | | Crippen Method |
| mcvol | 277.650 | ml/mol | McGowan Method |
| pc | 1497.67 | kPa | Joback Method |
| rinpol | 2499.00 | | NIST Webbook |
| rinpol | 2499.00 | | NIST Webbook |
| tb | 893.44 | K | Joback Method |
| tc | 1110.33 | K | Joback Method |
| tf | 519.81 | K | Joback Method |
| vc | 1.067 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 853.72 | J/mol×K | 893.44 | Joback Method |
| cpg | 867.20 | J/mol×K | 929.59 | Joback Method |
| cpg | 879.42 | J/mol×K | 965.74 | Joback Method |
| cpg | 890.41 | J/mol×K | 1001.88 | Joback Method |
| cpg | 900.19 | J/mol×K | 1038.03 | Joback Method |
| cpg | 908.81 | J/mol×K | 1074.18 | Joback Method |
| cpg | 916.30 | J/mol×K | 1110.33 | Joback Method |

# Sources

| | |
|---|---|
| **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=U377080&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |