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

**Inchi:** InChI=1S/C21H22F2O4/c22-18-8-3-1-6-16(18)12-14-26-20(24)10-5-11-21(25)27-15-13-1
**InchiKey:** ATRBGCAAEYMQBU-UHFFFAOYSA-N
**Formula:** C21H22F2O4
**SMILES:** O=C(CCCC(=O)OCCc1ccccc1F)OCCc1ccccc1F
**Mol. weight [g/mol]:** 376.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -525.96 | kJ/mol | Joback Method |
| hf | -908.47 | kJ/mol | Joback Method |
| hfus | 49.18 | kJ/mol | Joback Method |
| hvap | 84.89 | kJ/mol | Joback Method |
| log10ws | -5.21 | | Crippen Method |
| logp | 4.007 | | Crippen Method |
| mcvol | 277.650 | ml/mol | McGowan Method |
| pc | 1479.29 | kPa | Joback Method |
| rinpol | 2702.00 | | NIST Webbook |
| tb | 894.32 | K | Joback Method |
| tc | 1107.29 | K | Joback Method |
| tf | 549.81 | K | Joback Method |
| vc | 1.079 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 852.67 | J/mol×K | 894.32 | Joback Method |
| cpg | 865.98 | J/mol×K | 929.81 | Joback Method |
| cpg | 878.08 | J/mol×K | 965.31 | Joback Method |
| cpg | 889.02 | J/mol×K | 1000.80 | Joback Method |
| cpg | 898.83 | J/mol×K | 1036.30 | Joback Method |
| cpg | 907.54 | J/mol×K | 1071.79 | Joback Method |
| cpg | 915.18 | J/mol×K | 1107.29 | Joback Method |

# Sources

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|---|---|
| **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=U377099&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 |

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