# Glutaric acid, 3-methylbut-2-en-1-yl 3-fluorophenyl ester

**Inchi:** InChI=1S/C16H19FO4/c1-12(2)9-10-20-15(18)7-4-8-16(19)21-14-6-3-5-13(17)11-14/h3,5

**InchiKey:** YGGJMAUDOGVZKJ-UHFFFAOYSA-N

**Formula:** C16H19FO4

**SMILES:** CC(C)=CCOC(=O)CCCC(=O)Oc1cccc(F)c1

**Mol. weight [g/mol]:** 294.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -404.36 | kJ/mol | Joback Method |
| hf | -726.79 | kJ/mol | Joback Method |
| hfus | 38.39 | kJ/mol | Joback Method |
| hvap | 71.68 | kJ/mol | Joback Method |
| log10ws | -4.18 | | Crippen Method |
| logp | 3.411 | | Crippen Method |
| mcvol | 224.890 | ml/mol | McGowan Method |
| pc | 1835.69 | kPa | Joback Method |
| rinpol | 2032.00 | | NIST Webbook |
| rinpol | 2032.00 | | NIST Webbook |
| tb | 753.03 | K | Joback Method |
| tc | 956.57 | K | Joback Method |
| tf | 434.89 | K | Joback Method |
| vc | 0.871 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 631.35 | J/mol×K | 753.03 | Joback Method |
| cpg | 645.53 | J/mol×K | 786.95 | Joback Method |
| cpg | 658.79 | J/mol×K | 820.88 | Joback Method |
| cpg | 671.15 | J/mol×K | 854.80 | Joback Method |
| cpg | 682.63 | J/mol×K | 888.72 | Joback Method |
| cpg | 693.26 | J/mol×K | 922.64 | Joback Method |
| cpg | 703.07 | J/mol×K | 956.57 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392089&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 |

# 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 |