# Glutaric acid, tridec-2-yn-1-yl 3-fluorophenyl ester

**Inchi:** InChI=1S/C24H33FO4/c1-2-3-4-5-6-7-8-9-10-11-12-19-28-23(26)17-14-18-24(27)29-22-1

**InchiKey:** NRXBCZOPLLOXPX-UHFFFAOYSA-N

**Formula:** C24H33FO4

**SMILES:** CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1cccc(F)c1

**Mol. weight [g/mol]:** 404.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -205.87 | kJ/mol | Joback Method |
| hf | -727.04 | kJ/mol | Joback Method |
| hfus | 63.34 | kJ/mol | Joback Method |
| hvap | 91.60 | kJ/mol | Joback Method |
| log10ws | -7.47 | | Crippen Method |
| logp | 5.979 | | Crippen Method |
| mcvol | 333.310 | ml/mol | McGowan Method |
| pc | 1111.85 | kPa | Joback Method |
| rinpol | 2892.00 | | NIST Webbook |
| tb | 941.03 | K | Joback Method |
| tc | 1153.98 | K | Joback Method |
| tf | 650.19 | K | Joback Method |
| vc | 1.300 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1071.58 | J/mol×K | 941.03 | Joback Method |
| cpg | 1087.28 | J/mol×K | 976.52 | Joback Method |
| cpg | 1101.65 | J/mol×K | 1012.01 | Joback Method |
| cpg | 1114.74 | J/mol×K | 1047.50 | Joback Method |
| cpg | 1126.58 | J/mol×K | 1082.99 | Joback Method |
| cpg | 1137.21 | J/mol×K | 1118.49 | Joback Method |
| cpg | 1146.65 | J/mol×K | 1153.98 | 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=U392100&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |