# Glutaric acid, 3-fluorophenyl hexadecyl ester

**Inchi:** InChI=1S/C27H43FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-31-26(29)20-17-21-27(3
**InchiKey:** QETVOPGDGILNOT-UHFFFAOYSA-N
**Formula:** C27H43FO4
**SMILES:** CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(F)c1
**Mol. weight [g/mol]:** 450.63

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -383.41 | kJ/mol | Joback Method |
| hf | -1061.26 | kJ/mol | Joback Method |
| hfus | 67.99 | kJ/mol | Joback Method |
| hvap | 96.13 | kJ/mol | Joback Method |
| log10ws | -8.93 | | Crippen Method |
| logp | 7.926 | | Crippen Method |
| mcvol | 384.180 | ml/mol | McGowan Method |
| pc | 841.62 | kPa | Joback Method |
| rinpol | 3239.00 | | NIST Webbook |
| rinpol | 3239.00 | | NIST Webbook |
| tb | 1000.67 | K | Joback Method |
| tc | 1229.47 | K | Joback Method |
| tf | 577.90 | K | Joback Method |
| vc | 1.506 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1313.16 | J/mol×K | 1000.67 | Joback Method |
| cpg | 1331.08 | J/mol×K | 1038.80 | Joback Method |
| cpg | 1347.32 | J/mol×K | 1076.94 | Joback Method |
| cpg | 1361.94 | J/mol×K | 1115.07 | Joback Method |
| cpg | 1375.00 | J/mol×K | 1153.21 | Joback Method |
| cpg | 1386.57 | J/mol×K | 1191.34 | Joback Method |
| cpg | 1396.71 | J/mol×K | 1229.47 | Joback Method |

# Sources

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|---|---|
| **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=U359060&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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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