# Glutaric acid, 2-fluorophenyl cis-4-tert-butylcyclohexyl ester

**Inchi:** InChI=1S/C21H29FO4/c1-21(2,3)15-11-13-16(14-12-15)25-19(23)9-6-10-20(24)26-18-8-

**InchiKey:** QNOCRVOAUWZSEE-UHFFFAOYSA-N

**Formula:** C21H29FO4

**SMILES:** CC(C)(C)C1CCC(OC(=O)CCCC(=O)Oc2ccccc2F)CC1

**Mol. weight [g/mol]:** 364.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -414.35 | kJ/mol | Joback Method |
| hf | -912.19 | kJ/mol | Joback Method |
| hfus | 37.94 | kJ/mol | Joback Method |
| hvap | 81.60 | kJ/mol | Joback Method |
| log10ws | -5.94 | | Crippen Method |
| logp | 5.050 | | Crippen Method |
| mcvol | 288.780 | ml/mol | McGowan Method |
| pc | 1392.29 | kPa | Joback Method |
| rinpol | 2506.00 | | NIST Webbook |
| rinpol | 2506.00 | | NIST Webbook |
| tb | 875.04 | K | Joback Method |
| tc | 1094.03 | K | Joback Method |
| tf | 515.84 | K | Joback Method |
| vc | 1.091 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 944.39 | J/mol×K | 875.04 | Joback Method |
| cpg | 961.42 | J/mol×K | 911.54 | Joback Method |
| cpg | 976.93 | J/mol×K | 948.04 | Joback Method |
| cpg | 990.97 | J/mol×K | 984.54 | Joback Method |
| cpg | 1003.58 | J/mol×K | 1021.04 | Joback Method |
| cpg | 1014.83 | J/mol×K | 1057.54 | Joback Method |
| cpg | 1024.75 | J/mol×K | 1094.03 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393388&Units=SI |

# 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 |