# Glutaric acid, 2-fluorophenyl 1-naphthyl ester

**Inchi:** InChI=1S/C21H17FO4/c22-17-10-3-4-11-19(17)26-21(24)14-6-13-20(23)25-18-12-5-8-15
**InchiKey:** BMCJBOVHUOYDDL-UHFFFAOYSA-N
**Formula:** C21H17FO4
**SMILES:** O=C(CCCC(=O)Oc1cccc2ccccc12)Oc1ccccc1F
**Mol. weight [g/mol]:** 352.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -224.50 | kJ/mol | Joback Method |
| hf | -521.29 | kJ/mol | Joback Method |
| hfus | 43.12 | kJ/mol | Joback Method |
| hvap | 87.35 | kJ/mol | Joback Method |
| log10ws | -6.30 | | Crippen Method |
| logp | 4.660 | | Crippen Method |
| mcvol | 256.420 | ml/mol | McGowan Method |
| pc | 1874.03 | kPa | Joback Method |
| rinpol | 2930.00 | | NIST Webbook |
| rinpol | 2930.00 | | NIST Webbook |
| tb | 914.03 | K | Joback Method |
| tc | 1147.93 | K | Joback Method |
| tf | 581.92 | K | Joback Method |
| vc | 0.984 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 765.64 | J/mol×K | 914.03 | Joback Method |
| cpg | 777.79 | J/mol×K | 953.01 | Joback Method |
| cpg | 788.80 | J/mol×K | 992.00 | Joback Method |
| cpg | 798.76 | J/mol×K | 1030.98 | Joback Method |
| cpg | 807.73 | J/mol×K | 1069.96 | Joback Method |
| cpg | 815.78 | J/mol×K | 1108.95 | Joback Method |
| cpg | 822.98 | J/mol×K | 1147.93 | Joback Method |

# Sources

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|---|---|
| **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=U393335&Units=SI |

# 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 |