# Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-cyanophenyl ester

**Inchi:** InChI=1S/C15H13F4NO4/c16-14(17)15(18,19)9-23-12(21)2-1-3-13(22)24-11-6-4-10(8-20

**InchiKey:** TYAQIQMCBDWRMY-UHFFFAOYSA-N

**Formula:** C15H13F4NO4

**SMILES:** N#Cc1ccc(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)cc1

**Mol. weight [g/mol]:** 347.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -935.30 | kJ/mol | Joback Method |
| hf | -1251.06 | kJ/mol | Joback Method |
| hfus | 36.72 | kJ/mol | Joback Method |
| hvap | 75.76 | kJ/mol | Joback Method |
| log10ws | -4.14 | | Crippen Method |
| logp | 3.078 | | Crippen Method |
| mcvol | 221.790 | ml/mol | McGowan Method |
| pc | 1696.30 | kPa | Joback Method |
| rinpol | 2118.00 | | NIST Webbook |
| tb | 822.33 | K | Joback Method |
| tc | 1024.46 | K | Joback Method |
| tf | 496.84 | K | Joback Method |
| vc | 0.896 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 648.44 | J/mol×K | 822.33 | Joback Method |
| cpg | 658.74 | J/mol×K | 856.02 | Joback Method |
| cpg | 668.18 | J/mol×K | 889.71 | Joback Method |
| cpg | 676.79 | J/mol×K | 923.40 | Joback Method |
| cpg | 684.60 | J/mol×K | 957.09 | Joback Method |
| cpg | 691.64 | J/mol×K | 990.78 | Joback Method |
| cpg | 697.93 | J/mol×K | 1024.46 | 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=U393271&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 |