# Glutaric acid, 2,2,3,3-tetrafluoropropyl but-3-yn-2-yl ester

**Inchi:** InChI=1S/C12H14F4O4/c1-3-8(2)20-10(18)6-4-5-9(17)19-7-12(15,16)11(13)14/h1,8,11H

**InchiKey:** FHPXLBDMGDZCKP-UHFFFAOYSA-N

**Formula:** C12H14F4O4

**SMILES:** C#CC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)F

**Mol. weight [g/mol]:** 298.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -975.89 | kJ/mol | Joback Method |
| hf | -1292.46 | kJ/mol | Joback Method |
| hfus | 33.24 | kJ/mol | Joback Method |
| hvap | 55.14 | kJ/mol | Joback Method |
| log10ws | -3.11 | | Crippen Method |
| logp | 2.165 | | Crippen Method |
| mcvol | 193.300 | ml/mol | McGowan Method |
| pc | 1932.13 | kPa | Joback Method |
| rinpol | 1392.00 | | NIST Webbook |
| tb | 609.63 | K | Joback Method |
| tc | 782.64 | K | Joback Method |
| tf | 391.07 | K | Joback Method |
| vc | 0.766 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 509.27 | J/mol×K | 609.63 | Joback Method |
| cpg | 521.58 | J/mol×K | 638.47 | Joback Method |
| cpg | 533.24 | J/mol×K | 667.30 | Joback Method |
| cpg | 544.28 | J/mol×K | 696.14 | Joback Method |
| cpg | 554.70 | J/mol×K | 724.97 | Joback Method |
| cpg | 564.53 | J/mol×K | 753.81 | Joback Method |
| cpg | 573.78 | J/mol×K | 782.64 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393990&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |