# Glutaric acid, hex-4-yn-3-yl 1,1,1-trifluoroprop-2-yl ester

**Inchi:** InChI=1S/C14H19F3O4/c1-4-7-11(5-2)21-13(19)9-6-8-12(18)20-10(3)14(15,16)17/h10-1

**InchiKey:** JZFJTNXZHWECCJ-UHFFFAOYSA-N

**Formula:** C14H19F3O4

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

**Mol. weight [g/mol]:** 308.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -784.51 | kJ/mol | Joback Method |
| hf | -1157.23 | kJ/mol | Joback Method |
| hfus | 35.49 | kJ/mol | Joback Method |
| hvap | 62.70 | kJ/mol | Joback Method |
| log10ws | -4.09 | | Crippen Method |
| logp | 2.996 | | Crippen Method |
| mcvol | 219.710 | ml/mol | McGowan Method |
| pc | 1721.73 | kPa | Joback Method |
| rinpol | 1527.00 | | NIST Webbook |
| rinpol | 1527.00 | | NIST Webbook |
| tb | 675.00 | K | Joback Method |
| tc | 859.82 | K | Joback Method |
| tf | 472.15 | K | Joback Method |
| vc | 0.861 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 606.20 | J/mol×K | 675.00 | Joback Method |
| cpg | 620.44 | J/mol×K | 705.80 | Joback Method |
| cpg | 633.90 | J/mol×K | 736.61 | Joback Method |
| cpg | 646.59 | J/mol×K | 767.41 | Joback Method |
| cpg | 658.52 | J/mol×K | 798.21 | Joback Method |
| cpg | 669.72 | J/mol×K | 829.01 | Joback Method |
| cpg | 680.20 | J/mol×K | 859.82 | Joback Method |

# Sources

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|---|---|
| **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=U393654&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |