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

**Inchi:** InChI=1S/C14H17F5O4/c1-3-6-10(4-2)23-12(21)8-5-7-11(20)22-9-13(15,16)14(17,18)19/

**InchiKey:** YSQMZFOHFCXFCP-UHFFFAOYSA-N

**Formula:** C14H17F5O4

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

**Mol. weight [g/mol]:** 344.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1168.85 | kJ/mol | Joback Method |
| hf | -1552.92 | kJ/mol | Joback Method |
| hfus | 37.76 | kJ/mol | Joback Method |
| hvap | 60.16 | kJ/mol | Joback Method |
| log10ws | -4.29 | | Crippen Method |
| logp | 3.243 | | Crippen Method |
| mcvol | 223.250 | ml/mol | McGowan Method |
| pc | 1614.17 | kPa | Joback Method |
| rinpol | 1468.00 | | NIST Webbook |
| rinpol | 1468.00 | | NIST Webbook |
| tb | 670.75 | K | Joback Method |
| tc | 848.07 | K | Joback Method |
| tf | 490.75 | K | Joback Method |
| vc | 0.891 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 624.42 | J/mol×K | 670.75 | Joback Method |
| cpg | 637.77 | J/mol×K | 700.30 | Joback Method |
| cpg | 650.35 | J/mol×K | 729.86 | Joback Method |
| cpg | 662.18 | J/mol×K | 759.41 | Joback Method |
| cpg | 673.30 | J/mol×K | 788.96 | Joback Method |
| cpg | 683.73 | J/mol×K | 818.51 | Joback Method |
| cpg | 693.50 | J/mol×K | 848.07 | Joback Method |

# Sources

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|---|---|
| **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=U393670&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |