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

**Inchi:** InChI=1S/C14H21F3O4/c1-3-4-5-6-10-20-12(18)8-7-9-13(19)21-11(2)14(15,16)17/h3-4,1

**InchiKey:** YGHNWMIITOXCGI-ONEGZZNKSA-N

**Formula:** C14H21F3O4

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

**Mol. weight [g/mol]:** 310.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -904.65 | kJ/mol | Joback Method |
| hf | -1307.03 | kJ/mol | Joback Method |
| hfus | 36.09 | kJ/mol | Joback Method |
| hvap | 60.89 | kJ/mol | Joback Method |
| log10ws | -4.04 | | Crippen Method |
| logp | 3.550 | | Crippen Method |
| mcvol | 224.010 | ml/mol | McGowan Method |
| pc | 1567.23 | kPa | Joback Method |
| rinpol | 1574.00 | | NIST Webbook |
| rinpol | 1574.00 | | NIST Webbook |
| tb | 670.60 | K | Joback Method |
| tc | 843.97 | K | Joback Method |
| tf | 375.97 | K | Joback Method |
| vc | 0.884 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 627.05 | J/mol×K | 670.60 | Joback Method |
| cpg | 641.24 | J/mol×K | 699.50 | Joback Method |
| cpg | 654.68 | J/mol×K | 728.39 | Joback Method |
| cpg | 667.42 | J/mol×K | 757.29 | Joback Method |
| cpg | 679.45 | J/mol×K | 786.18 | Joback Method |
| cpg | 690.82 | J/mol×K | 815.08 | Joback Method |
| cpg | 701.54 | J/mol×K | 843.97 | Joback Method |

# Sources

| | |
|---|---|
| **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=U405294&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 |