# Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl hex-4-yn-3-yl ester

**Inchi:** InChI=1S/C16H18F8O4/c1-3-6-10(4-2)28-12(26)8-5-7-11(25)27-9-14(19,20)16(23,24)15(21,22)13(17)18/h10,13H,4-5,7-9H2,1-2H3

**InchiKey:** NNVKMOXZPMEGOK-UHFFFAOYSA-N

**Formula:** C16H18F8O4

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

**Mol. weight [g/mol]:** 426.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1736.04 | kJ/mol | Joback Method |
| hf | -2196.56 | kJ/mol | Joback Method |
| hfus | 41.24 | kJ/mol | Joback Method |
| hvap | 60.47 | kJ/mol | Joback Method |
| log10ws | -5.41 | | Crippen Method |
| logp | 4.216 | | Crippen Method |
| mcvol | 256.740 | ml/mol | McGowan Method |
| pc | 1285.59 | kPa | Joback Method |
| rinpol | 1684.00 | | NIST Webbook |
| rinpol | 1684.00 | | NIST Webbook |
| tb | 710.65 | K | Joback Method |
| tc | 881.82 | K | Joback Method |
| tf | 502.48 | K | Joback Method |
| vc | 1.040 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 758.36 | J/mol×K | 710.65 | Joback Method |
| cpg | 771.71 | J/mol×K | 739.18 | Joback Method |
| cpg | 784.24 | J/mol×K | 767.71 | Joback Method |
| cpg | 795.99 | J/mol×K | 796.24 | Joback Method |
| cpg | 806.99 | J/mol×K | 824.77 | Joback Method |
| cpg | 817.30 | J/mol×K | 853.30 | Joback Method |
| cpg | 826.94 | J/mol×K | 881.82 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393971&Units=SI |

# 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 |