# Fumaric acid, di(2,2,3,3,4,4,5,5-octafluoropentyl) ester

**Inchi:** InChI=1S/C14H8F16O4/c15-7(16)11(23,24)13(27,28)9(19,20)3-33-5(31)1-2-6(32)34-4-10

**InchiKey:** GJKYQRGXEQSQOI-OWOJBTEDSA-N

**Formula:** C14H8F16O4

**SMILES:** O=C(C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 544.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -3425.42 | kJ/mol | Joback Method |
| hf | -3905.49 | kJ/mol | Joback Method |
| hfus | 35.54 | kJ/mol | Joback Method |
| hvap | 43.40 | kJ/mol | Joback Method |
| log10ws | -5.77 | | Crippen Method |
| logp | 4.971 | | Crippen Method |
| mcvol | 247.020 | ml/mol | McGowan Method |
| pc | 1105.21 | kPa | Joback Method |
| rinpol | 1434.00 | | NIST Webbook |
| rinpol | 1434.00 | | NIST Webbook |
| tb | 644.52 | K | Joback Method |
| tc | 792.42 | K | Joback Method |
| tf | 380.74 | K | Joback Method |
| vc | 1.058 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 745.65 | J/mol×K | 644.52 | Joback Method |
| cpg | 756.78 | J/mol×K | 669.17 | Joback Method |
| cpg | 767.09 | J/mol×K | 693.82 | Joback Method |
| cpg | 776.65 | J/mol×K | 718.47 | Joback Method |
| cpg | 785.50 | J/mol×K | 743.12 | Joback Method |
| cpg | 793.71 | J/mol×K | 767.77 | Joback Method |
| cpg | 801.31 | J/mol×K | 792.42 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348797&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 |

# 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 |