# Fumaric acid, 4-octyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C17H22F8O4/c1-3-5-7-11(6-4-2)29-13(27)9-8-12(26)28-10-15(20,21)17(24,25)

**InchiKey:** HEOGZYCPKMKLOT-CMDGGOBGSA-N

**Formula:** C17H22F8O4

**SMILES:** CCCCC(CCC)OC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 442.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1850.20 | kJ/mol | Joback Method |
| hf | -2372.28 | kJ/mol | Joback Method |
| hfus | 40.91 | kJ/mol | Joback Method |
| hvap | 60.51 | kJ/mol | Joback Method |
| log10ws | -5.89 | | Crippen Method |
| logp | 5.159 | | Crippen Method |
| mcvol | 275.130 | ml/mol | McGowan Method |
| pc | 1116.31 | kPa | Joback Method |
| rinpol | 1740.00 | | NIST Webbook |
| rinpol | 1740.00 | | NIST Webbook |
| tb | 728.69 | K | Joback Method |
| tc | 896.59 | K | Joback Method |
| tf | 402.57 | K | Joback Method |
| vc | 1.115 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 835.97 | J/mol×K | 728.69 | Joback Method |
| cpg | 850.12 | J/mol×K | 756.67 | Joback Method |
| cpg | 863.42 | J/mol×K | 784.66 | Joback Method |
| cpg | 875.93 | J/mol×K | 812.64 | Joback Method |
| cpg | 887.69 | J/mol×K | 840.62 | Joback Method |
| cpg | 898.76 | J/mol×K | 868.61 | Joback Method |
| cpg | 909.18 | J/mol×K | 896.59 | Joback Method |

# Sources

| | |
|---|---|
| **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=U405620&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 |

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