# Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-fluorophenyl ester

**Inchi:** InChI=1S/C16H13F9O4/c17-9-3-1-4-10(7-9)29-12(27)6-2-5-11(26)28-8-14(20,21)16(24,2

**InchiKey:** CWTWUJNSRFMKNC-UHFFFAOYSA-N

**Formula:** C16H13F9O4

**SMILES:** O=C(CCCC(=O)Oc1cccc(F)c1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 440.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2028.43 | kJ/mol | Joback Method |
| hf | -2434.63 | kJ/mol | Joback Method |
| hfus | 38.38 | kJ/mol | Joback Method |
| hvap | 60.83 | kJ/mol | Joback Method |
| log10ws | -5.58 | | Crippen Method |
| logp | 4.616 | | Crippen Method |
| mcvol | 243.350 | ml/mol | McGowan Method |
| pc | 1386.08 | kPa | Joback Method |
| rinpol | 1816.00 | | NIST Webbook |
| rinpol | 1816.00 | | NIST Webbook |
| tb | 733.02 | K | Joback Method |
| tc | 908.43 | K | Joback Method |
| tf | 450.91 | K | Joback Method |
| vc | 0.995 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 725.73 | J/mol×K | 733.02 | Joback Method |
| cpg | 737.57 | J/mol×K | 762.26 | Joback Method |
| cpg | 748.56 | J/mol×K | 791.49 | Joback Method |
| cpg | 758.76 | J/mol×K | 820.73 | Joback Method |
| cpg | 768.22 | J/mol×K | 849.96 | Joback Method |
| cpg | 776.98 | J/mol×K | 879.20 | Joback Method |
| cpg | 785.09 | J/mol×K | 908.43 | Joback Method |

# Sources

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|---|---|
| **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=U392085&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 |