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

**Inchi:** InChI=1S/C16H12F8O5/c1-27-9-4-2-3-5-10(9)29-12(26)7-6-11(25)28-8-14(19,20)16(23,2

**InchiKey:** JUJIOLJYRDJYTD-VOTSOKGWSA-N

**Formula:** C16H12F8O5

**SMILES:** COc1ccccc1OC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 436.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1858.40 | kJ/mol | Joback Method |
| hf | -2253.52 | kJ/mol | Joback Method |
| hfus | 36.69 | kJ/mol | Joback Method |
| hvap | 64.02 | kJ/mol | Joback Method |
| log10ws | -4.81 | | Crippen Method |
| logp | 3.871 | | Crippen Method |
| mcvol | 243.150 | ml/mol | McGowan Method |
| pc | 1472.49 | kPa | Joback Method |
| rinpol | 1923.00 | | NIST Webbook |
| rinpol | 1923.00 | | NIST Webbook |
| tb | 760.33 | K | Joback Method |
| tc | 945.01 | K | Joback Method |
| tf | 467.47 | K | Joback Method |
| vc | 0.975 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 719.73 | J/mol×K | 760.33 | Joback Method |
| cpg | 731.00 | J/mol×K | 791.11 | Joback Method |
| cpg | 741.43 | J/mol×K | 821.89 | Joback Method |
| cpg | 751.05 | J/mol×K | 852.67 | Joback Method |
| cpg | 759.92 | J/mol×K | 883.45 | Joback Method |
| cpg | 768.10 | J/mol×K | 914.23 | Joback Method |
| cpg | 775.64 | J/mol×K | 945.01 | 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=U405927&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 |