# Fumaric acid, isobutyl pentafluorophenyl ester

**Inchi:** InChI=1S/C14H11F5O4/c1-6(2)5-22-7(20)3-4-8(21)23-14-12(18)10(16)9(15)11(17)13(14
**InchiKey:** CPCPEQPLOBNXGY-ONEGZZNKSA-N
**Formula:** C14H11F5O4
**SMILES:** CC(C)COC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 338.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1232.85 | kJ/mol | Joback Method |
| hf | -1511.32 | kJ/mol | Joback Method |
| hfus | 41.76 | kJ/mol | Joback Method |
| hvap | 66.14 | kJ/mol | Joback Method |
| log10ws | -4.43 | | Crippen Method |
| logp | 3.043 | | Crippen Method |
| mcvol | 203.790 | ml/mol | McGowan Method |
| pc | 1766.90 | kPa | Joback Method |
| rinpol | 1601.00 | | NIST Webbook |
| tb | 723.95 | K | Joback Method |
| tc | 908.85 | K | Joback Method |
| tf | 463.75 | K | Joback Method |
| vc | 0.824 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 552.01 | J/mol×K | 723.95 | Joback Method |
| cpg | 563.05 | J/mol×K | 754.77 | Joback Method |
| cpg | 573.44 | J/mol×K | 785.58 | Joback Method |
| cpg | 583.21 | J/mol×K | 816.40 | Joback Method |
| cpg | 592.33 | J/mol×K | 847.22 | Joback Method |
| cpg | 600.83 | J/mol×K | 878.03 | Joback Method |
| cpg | 608.68 | J/mol×K | 908.85 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348095&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 |