# Methyl 2-hydroxy-4-methoxybenzoate, O-pentafluoropropionyl-

**Inchi:** InChI=1S/C12H9F5O5/c1-20-6-3-4-7(9(18)21-2)8(5-6)22-10(19)11(13,14)12(15,16)17/h3

**InchiKey:** ZATMWZCIBDRJDZ-UHFFFAOYSA-N

**Formula:** C12H9F5O5

**SMILES:** COC(=O)c1ccc(OC)cc1OC(=O)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 328.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1397.90 | kJ/mol | Joback Method |
| hf | -1697.29 | kJ/mol | Joback Method |
| hfus | 27.43 | kJ/mol | Joback Method |
| hvap | 59.95 | kJ/mol | Joback Method |
| log10ws | -3.54 | | Crippen Method |
| logp | 2.585 | | Crippen Method |
| mcvol | 185.780 | ml/mol | McGowan Method |
| pc | 2102.27 | kPa | Joback Method |
| rinpol | 1492.00 | | NIST Webbook |
| rinpol | 1492.00 | | NIST Webbook |
| tb | 675.49 | K | Joback Method |
| tc | 865.86 | K | Joback Method |
| tf | 450.80 | K | Joback Method |
| vc | 0.734 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 506.81 | J/mol×K | 675.49 | Joback Method |
| cpg | 517.78 | J/mol×K | 707.22 | Joback Method |
| cpg | 527.99 | J/mol×K | 738.95 | Joback Method |
| cpg | 537.46 | J/mol×K | 770.68 | Joback Method |
| cpg | 546.22 | J/mol×K | 802.41 | Joback Method |
| cpg | 554.26 | J/mol×K | 834.14 | Joback Method |
| cpg | 561.63 | J/mol×K | 865.86 | 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=U374793&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 |