# 2,6-Dimethoxyphenol, pentafluoropropionate

**Inchi:** InChI=1S/C11H9F5O4/c1-18-6-4-3-5-7(19-2)8(6)20-9(17)10(12,13)11(14,15)16/h3-5H,1-
**InchiKey:** IWWKATRLWJSPNZ-UHFFFAOYSA-N
**Formula:** C11H9F5O4
**SMILES:** COc1cccc(OC)c1OC(=O)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 300.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1277.40 | kJ/mol | Joback Method |
| hf | -1564.07 | kJ/mol | Joback Method |
| hfus | 23.24 | kJ/mol | Joback Method |
| hvap | 50.98 | kJ/mol | Joback Method |
| log10ws | -3.42 | | Crippen Method |
| logp | 2.807 | | Crippen Method |
| mcvol | 170.120 | ml/mol | McGowan Method |
| pc | 2167.36 | kPa | Joback Method |
| rinpol | 1304.00 | | NIST Webbook |
| tb | 598.74 | K | Joback Method |
| tc | 783.55 | K | Joback Method |
| tf | 389.60 | K | Joback Method |
| vc | 0.671 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 442.65 | J/mol×K | 598.74 | Joback Method |
| cpg | 454.35 | J/mol×K | 629.54 | Joback Method |
| cpg | 465.35 | J/mol×K | 660.34 | Joback Method |
| cpg | 475.67 | J/mol×K | 691.15 | Joback Method |
| cpg | 485.32 | J/mol×K | 721.95 | Joback Method |
| cpg | 494.33 | J/mol×K | 752.75 | Joback Method |
| cpg | 502.70 | J/mol×K | 783.55 | 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=U374279&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 |