# 4-Isopropylphenol, pentafluorobenzoyl ester

**Inchi:** InChI=1S/C16H11F5O2/c1-7(2)8-3-5-9(6-4-8)23-16(22)10-11(17)13(19)15(21)14(20)12(1
**InchiKey:** CVZZJJGBQQGIQE-UHFFFAOYSA-N
**Formula:** C16H11F5O2
**SMILES:** CC(C)c1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
**Mol. weight [g/mol]:** 330.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -959.53 | kJ/mol | Joback Method |
| hf | -1199.96 | kJ/mol | Joback Method |
| hfus | 37.61 | kJ/mol | Joback Method |
| hvap | 64.42 | kJ/mol | Joback Method |
| log10ws | -6.40 | | Crippen Method |
| logp | 4.725 | | Crippen Method |
| mcvol | 205.070 | ml/mol | McGowan Method |
| pc | 1806.16 | kPa | Joback Method |
| rinpol | 1737.50 | | NIST Webbook |
| rinpol | 1737.50 | | NIST Webbook |
| rinpol | 1740.10 | | NIST Webbook |
| rinpol | 1742.90 | | NIST Webbook |
| tb | 720.92 | K | Joback Method |
| tc | 919.23 | K | Joback Method |
| tf | 458.15 | K | Joback Method |
| vc | 0.824 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 552.85 | J/mol×K | 720.92 | Joback Method |
| cpg | 565.19 | J/mol×K | 753.97 | Joback Method |
| cpg | 576.75 | J/mol×K | 787.02 | Joback Method |
| cpg | 587.52 | J/mol×K | 820.08 | Joback Method |
| cpg | 597.52 | J/mol×K | 853.13 | Joback Method |
| cpg | 606.77 | J/mol×K | 886.18 | Joback Method |

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|---|---|---|---|---|
| cpg | 615.26 | J/mol×K | 919.23 | Joback Method |

# Sources

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|---|---|
| **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=R433322&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |