# 2,3,6-Trimethylphenol, pentafluorobenzoyl ester

**Inchi:** InChI=1S/C16H11F5O2/c1-6-4-5-7(2)15(8(6)3)23-16(22)9-10(17)12(19)14(21)13(20)11(9

**InchiKey:** UPZDETHWGKIHJR-UHFFFAOYSA-N

**Formula:** C16H11F5O2

**SMILES:** Cc1ccc(C)c(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c1C

**Mol. weight [g/mol]:** 330.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -976.35 | kJ/mol | Joback Method |
| hf | -1217.62 | kJ/mol | Joback Method |
| hfus | 40.35 | kJ/mol | Joback Method |
| hvap | 66.13 | kJ/mol | Joback Method |
| log10ws | -6.64 | | Crippen Method |
| logp | 4.527 | | Crippen Method |
| mcvol | 205.070 | ml/mol | McGowan Method |
| pc | 1749.21 | kPa | Joback Method |
| rinpol | 1756.90 | | NIST Webbook |
| rinpol | 1761.10 | | NIST Webbook |
| rinpol | 1766.70 | | NIST Webbook |
| rinpol | 1756.90 | | NIST Webbook |
| tb | 731.32 | K | Joback Method |
| tc | 928.38 | K | Joback Method |
| tf | 498.19 | K | Joback Method |
| vc | 0.830 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 549.91 | J/mol×K | 731.32 | Joback Method |
| cpg | 561.85 | J/mol×K | 764.16 | Joback Method |
| cpg | 573.08 | J/mol×K | 797.01 | Joback Method |
| cpg | 583.57 | J/mol×K | 829.85 | Joback Method |
| cpg | 593.34 | J/mol×K | 862.69 | Joback Method |
| cpg | 602.38 | J/mol×K | 895.54 | Joback Method |

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|---|---|---|---|---|
| cpg | 610.69 | J/mol×K | 928.38 | 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=R433000&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 |