# Benzoic acid, 3-methyl-, pentafluorophenyl ester

**Inchi:** InChI=1S/C14H7F5O2/c1-6-3-2-4-7(5-6)14(20)21-13-11(18)9(16)8(15)10(17)12(13)19/h2

**InchiKey:** KBTKEDPFFVPPMU-UHFFFAOYSA-N

**Formula:** C14H7F5O2

**SMILES:** Cc1cccc(C(=O)Oc2c(F)c(F)c(F)c(F)c2F)c1

**Mol. weight [g/mol]:** 302.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -973.93 | kJ/mol | Joback Method |
| hf | -1153.40 | kJ/mol | Joback Method |
| hfus | 35.95 | kJ/mol | Joback Method |
| hvap | 60.35 | kJ/mol | Joback Method |
| log10ws | -5.69 | | Crippen Method |
| logp | 3.910 | | Crippen Method |
| mcvol | 176.890 | ml/mol | McGowan Method |
| pc | 2125.60 | kPa | Joback Method |
| rinpol | 1600.00 | | NIST Webbook |
| rinpol | 1600.00 | | NIST Webbook |
| tb | 675.60 | K | Joback Method |
| tc | 874.76 | K | Joback Method |
| tf | 450.61 | K | Joback Method |
| vc | 0.718 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 449.69 | J/mol×K | 675.60 | Joback Method |
| cpg | 460.72 | J/mol×K | 708.79 | Joback Method |
| cpg | 471.08 | J/mol×K | 741.99 | Joback Method |
| cpg | 480.77 | J/mol×K | 775.18 | Joback Method |
| cpg | 489.80 | J/mol×K | 808.37 | Joback Method |
| cpg | 498.17 | J/mol×K | 841.57 | Joback Method |
| cpg | 505.88 | J/mol×K | 874.76 | 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=U355707&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 |