# 3-Fluorobenzoic acid, 2-methylpentyl ester

**Inchi:** InChI=1S/C13H17FO2/c1-3-5-10(2)9-16-13(15)11-6-4-7-12(14)8-11/h4,6-8,10H,3,5,9H2,
**InchiKey:** POAIQFAYNHZCNV-UHFFFAOYSA-N
**Formula:** C13H17FO2
**SMILES:** CCCC(C)COC(=O)c1cccc(F)c1
**Mol. weight [g/mol]:** 224.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -269.81 | kJ/mol | Joback Method |
| hf | -532.78 | kJ/mol | Joback Method |
| hfus | 25.42 | kJ/mol | Joback Method |
| hvap | 55.42 | kJ/mol | Joback Method |
| log10ws | -3.90 | | Crippen Method |
| logp | 3.419 | | Crippen Method |
| mcvol | 179.480 | ml/mol | McGowan Method |
| pc | 2181.56 | kPa | Joback Method |
| rinpol | 1539.00 | | NIST Webbook |
| tb | 603.62 | K | Joback Method |
| tc | 802.32 | K | Joback Method |
| tf | 332.96 | K | Joback Method |
| vc | 0.692 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 451.56 | J/mol×K | 603.62 | Joback Method |
| cpg | 466.76 | J/mol×K | 636.74 | Joback Method |
| cpg | 481.13 | J/mol×K | 669.85 | Joback Method |
| cpg | 494.70 | J/mol×K | 702.97 | Joback Method |
| cpg | 507.49 | J/mol×K | 736.09 | Joback Method |
| cpg | 519.51 | J/mol×K | 769.21 | Joback Method |
| cpg | 530.78 | J/mol×K | 802.32 | 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=U355663&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 |