# 2-Ethylbutyric acid, 4-fluoro-2-methoxyphenyl ester

**Inchi:** InChI=1S/C13H17FO3/c1-4-9(5-2)13(15)17-11-7-6-10(14)8-12(11)16-3/h6-9H,4-5H2,1-3

**InchiKey:** QZGLLTJQEQEQJH-UHFFFAOYSA-N

**Formula:** C13H17FO3

**SMILES:** CCC(CC)C(=O)Oc1ccc(F)cc1OC

**Mol. weight [g/mol]:** 240.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -384.44 | kJ/mol | Joback Method |
| hf | -676.47 | kJ/mol | Joback Method |
| hfus | 26.22 | kJ/mol | Joback Method |
| hvap | 58.49 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 3.176 | | Crippen Method |
| mcvol | 185.350 | ml/mol | McGowan Method |
| pc | 2117.78 | kPa | Joback Method |
| rinpol | 1559.00 | | NIST Webbook |
| rinpol | 1559.00 | | NIST Webbook |
| tb | 631.02 | K | Joback Method |
| tc | 828.98 | K | Joback Method |
| tf | 367.71 | K | Joback Method |
| vc | 0.710 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 477.44 | J/mol×K | 631.02 | Joback Method |
| cpg | 492.16 | J/mol×K | 664.01 | Joback Method |
| cpg | 506.11 | J/mol×K | 697.01 | Joback Method |
| cpg | 519.31 | J/mol×K | 730.00 | Joback Method |
| cpg | 531.75 | J/mol×K | 762.99 | Joback Method |
| cpg | 543.44 | J/mol×K | 795.98 | Joback Method |
| cpg | 554.37 | J/mol×K | 828.98 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370922&Units=SI |

# 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 |