# 2-Fluorobenzoic acid, 3-ethylphenyl ester

**Inchi:** InChI=1S/C15H13FO2/c1-2-11-6-5-7-12(10-11)18-15(17)13-8-3-4-9-14(13)16/h3-10H,2H
**InchiKey:** DIANMQIKLBLKOI-UHFFFAOYSA-N
**Formula:** C15H13FO2
**SMILES:** CCc1cccc(OC(=O)c2ccccc2F)c1
**Mol. weight [g/mol]:** 244.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -147.75 | kJ/mol | Joback Method |
| hf | -343.72 | kJ/mol | Joback Method |
| hfus | 27.78 | kJ/mol | Joback Method |
| hvap | 63.20 | kJ/mol | Joback Method |
| log10ws | -4.69 | | Crippen Method |
| logp | 3.607 | | Crippen Method |
| mcvol | 183.900 | ml/mol | McGowan Method |
| pc | 2438.65 | kPa | Joback Method |
| rinpol | 1932.00 | | NIST Webbook |
| tb | 681.48 | K | Joback Method |
| tc | 910.11 | K | Joback Method |
| tf | 409.44 | K | Joback Method |
| vc | 0.702 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 472.85 | J/mol×K | 681.48 | Joback Method |
| cpg | 487.50 | J/mol×K | 719.58 | Joback Method |
| cpg | 501.06 | J/mol×K | 757.69 | Joback Method |
| cpg | 513.60 | J/mol×K | 795.79 | Joback Method |
| cpg | 525.13 | J/mol×K | 833.90 | Joback Method |
| cpg | 535.70 | J/mol×K | 872.00 | Joback Method |
| cpg | 545.35 | J/mol×K | 910.11 | 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=U354705&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 |