# 2-Fluorobenzoic acid, 3-methylbut-2-enyl ester

**Inchi:** InChI=1S/C12H13FO2/c1-9(2)7-8-15-12(14)10-5-3-4-6-11(10)13/h3-7H,8H2,1-2H3
**InchiKey:** MEDMSMBQEOOHBM-UHFFFAOYSA-N
**Formula:** C12H13FO2
**SMILES:** CC(C)=CCOC(=O)c1ccccc1F
**Mol. weight [g/mol]:** 208.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -204.12 | kJ/mol | Joback Method |
| hf | -399.43 | kJ/mol | Joback Method |
| hfus | 25.25 | kJ/mol | Joback Method |
| hvap | 53.62 | kJ/mol | Joback Method |
| log10ws | -3.57 | | Crippen Method |
| logp | 2.949 | | Crippen Method |
| mcvol | 161.090 | ml/mol | McGowan Method |
| pc | 2510.03 | kPa | Joback Method |
| rinpol | 1475.00 | | NIST Webbook |
| tb | 585.22 | K | Joback Method |
| tc | 794.67 | K | Joback Method |
| tf | 317.65 | K | Joback Method |
| vc | 0.623 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 381.89 | J/mol×K | 585.22 | Joback Method |
| cpg | 395.78 | J/mol×K | 620.13 | Joback Method |
| cpg | 408.85 | J/mol×K | 655.04 | Joback Method |
| cpg | 421.14 | J/mol×K | 689.94 | Joback Method |
| cpg | 432.66 | J/mol×K | 724.85 | Joback Method |
| cpg | 443.46 | J/mol×K | 759.76 | Joback Method |
| cpg | 453.56 | J/mol×K | 794.67 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U299162&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |