# 3-Ethylphenol, O-pentafluoropropionyl-

**Inchi:** InChI=1S/C11H9F5O2/c1-2-7-4-3-5-8(6-7)18-9(17)10(12,13)11(14,15)16/h3-6H,2H2,1H3
**InchiKey:** YTCZUNLWTSOWCF-UHFFFAOYSA-N
**Formula:** C11H9F5O2
**SMILES:** CCc1cccc(OC(=O)C(F)(F)C(F)(F)F)c1
**Mol. weight [g/mol]:** 268.18

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1057.77 | kJ/mol | Joback Method |
| hf | -1288.16 | kJ/mol | Joback Method |
| hfus | 21.26 | kJ/mol | Joback Method |
| hvap | 45.50 | kJ/mol | Joback Method |
| log10ws | -3.98 | | Crippen Method |
| logp | 3.352 | | Crippen Method |
| mcvol | 158.380 | ml/mol | McGowan Method |
| pc | 2269.73 | kPa | Joback Method |
| rinpol | 1068.00 | | NIST Webbook |
| rinpol | 1068.00 | | NIST Webbook |
| tb | 548.92 | K | Joback Method |
| tc | 734.93 | K | Joback Method |
| tf | 332.62 | K | Joback Method |
| vc | 0.635 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 394.09 | J/mol×K | 548.92 | Joback Method |
| cpg | 406.67 | J/mol×K | 579.92 | Joback Method |
| cpg | 418.41 | J/mol×K | 610.92 | Joback Method |
| cpg | 429.35 | J/mol×K | 641.93 | Joback Method |
| cpg | 439.53 | J/mol×K | 672.93 | Joback Method |
| cpg | 449.00 | J/mol×K | 703.93 | Joback Method |
| cpg | 457.78 | J/mol×K | 734.93 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U374274&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 |