# Benzene, 1-fluoro-3-ethyl

**Inchi:** InChI=1S/C8H9F/c1-2-7-4-3-5-8(9)6-7/h3-6H,2H2,1H3
**InchiKey:** ZEWGMOQWTWMZMZ-UHFFFAOYSA-N
**Formula:** C8H9F
**SMILES:** CCc1cccc(F)c1
**Mol. weight [g/mol]:** 124.16

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -75.55 | kJ/mol | Joback Method |
| hf | -179.50 | kJ/mol | Joback Method |
| hfus | 13.21 | kJ/mol | Joback Method |
| hvap | 35.52 | kJ/mol | Joback Method |
| log10ws | -2.61 | | Crippen Method |
| logp | 2.388 | | Crippen Method |
| mcvol | 101.590 | ml/mol | McGowan Method |
| pc | 3399.94 | kPa | Joback Method |
| rinpol | 879.00 | | NIST Webbook |
| rinpol | 879.00 | | NIST Webbook |
| tb | 413.37 | K | Joback Method |
| tc | 612.69 | K | Joback Method |
| tf | 219.45 | K | Joback Method |
| vc | 0.394 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 184.90 | J/mol×K | 413.37 | Joback Method |
| cpg | 196.54 | J/mol×K | 446.59 | Joback Method |
| cpg | 207.57 | J/mol×K | 479.81 | Joback Method |
| cpg | 218.03 | J/mol×K | 513.03 | Joback Method |
| cpg | 227.93 | J/mol×K | 546.25 | Joback Method |
| cpg | 237.29 | J/mol×K | 579.47 | Joback Method |
| cpg | 246.13 | J/mol×K | 612.69 | Joback Method |

# Sources

| | |
|---|---|
| **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=R636318&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |

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