# Benzene, 2-fluoro-1,4-bis (1-methylethyl)-

**Inchi:** InChI=1S/C12H17F/c1-8(2)10-5-6-11(9(3)4)12(13)7-10/h5-9H,1-4H3
**InchiKey:** NTUDGJSTIQYBPG-UHFFFAOYSA-N
**Formula:** C12H17F
**SMILES:** CC(C)c1ccc(C(C)C)c(F)c1
**Mol. weight [g/mol]:** 180.26
**CAS:** 87591-03-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -56.38 | kJ/mol | Joback Method |
| hf | -284.09 | kJ/mol | Joback Method |
| hfus | 16.13 | kJ/mol | Joback Method |
| hvap | 44.31 | kJ/mol | Joback Method |
| log10ws | -4.17 | | Crippen Method |
| logp | 4.072 | | Crippen Method |
| mcvol | 157.950 | ml/mol | McGowan Method |
| pc | 2271.90 | kPa | Joback Method |
| tb | 508.99 | K | Joback Method |
| tc | 709.13 | K | Joback Method |
| tf | 247.05 | K | Joback Method |
| vc | 0.606 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 355.45 | J/mol×K | 508.99 | Joback Method |
| cpg | 371.64 | J/mol×K | 542.35 | Joback Method |
| cpg | 387.01 | J/mol×K | 575.70 | Joback Method |
| cpg | 401.59 | J/mol×K | 609.06 | Joback Method |
| cpg | 415.40 | J/mol×K | 642.41 | Joback Method |
| cpg | 428.47 | J/mol×K | 675.77 | Joback Method |
| cpg | 440.83 | J/mol×K | 709.13 | Joback Method |

# Sources

| | |
|---|---|
| **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=C87591035&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |