# Benzene, 1-(2,2-dimethyl-1-methylenepropyl)-3-fluoro-

**Inchi:** InChI=1S/C12H15F/c1-9(12(2,3)4)10-6-5-7-11(13)8-10/h5-8H,1H2,2-4H3
**InchiKey:** AGFFWVOXOGOEID-UHFFFAOYSA-N
**Formula:** C12H15F
**SMILES:** C=C(c1cccc(F)c1)C(C)(C)C
**Mol. weight [g/mol]:** 178.25
**CAS:** 146558-44-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 838.80 | kJ/mol | NIST Webbook |
| basg | 809.90 | kJ/mol | NIST Webbook |
| gf | 40.26 | kJ/mol | Joback Method |
| hf | -155.17 | kJ/mol | Joback Method |
| hfus | 13.56 | kJ/mol | Joback Method |
| hvap | 42.54 | kJ/mol | Joback Method |
| log10ws | -4.06 | | Crippen Method |
| logp | 3.885 | | Crippen Method |
| mcvol | 153.650 | ml/mol | McGowan Method |
| pc | 2419.50 | kPa | Joback Method |
| tb | 498.22 | K | Joback Method |
| tc | 709.15 | K | Joback Method |
| tf | 251.23 | K | Joback Method |
| vc | 0.589 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 338.89 | J/mol×K | 498.22 | Joback Method |
| cpg | 355.54 | J/mol×K | 533.37 | Joback Method |
| cpg | 371.11 | J/mol×K | 568.53 | Joback Method |
| cpg | 385.64 | J/mol×K | 603.68 | Joback Method |
| cpg | 399.21 | J/mol×K | 638.84 | Joback Method |
| cpg | 411.87 | J/mol×K | 673.99 | Joback Method |
| cpg | 423.67 | J/mol×K | 709.15 | Joback Method |

# Sources

| | |
|---|---|
| **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=C146558443&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |

Latest version available from:
https://www.chemeo.com/cid/45-437-7/Benzene-1-2-2-dimethyl-1-methylenepropyl-3-fluoro.pdf
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