# Benzene, 1-fluoro-3-methyl-

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|---|---|
| **Other names:** | 1-FLUORO-3-METHYLBENZENE |
| | 1-Methyl-3-fluorobenzene |
| | 3-FLUOROTOLUENE |
| | Toluene, 3-fluoro |
| | Toluene, m-fluoro- |
| | UN 2388 |
| | m-Fluorotoluene |
| | meta-Fluorotoluene |
| **Inchi:** | InChI=1S/C7H7F/c1-6-3-2-4-7(8)5-6/h2-5H,1H3 |
| **InchiKey:** | BTQZKHUEUDPRST-UHFFFAOYSA-N |
| **Formula:** | C7H7F |
| **SMILES:** | Cc1cccc(F)c1 |
| **Mol. weight [g/mol]:** | 110.13 |
| **CAS:** | 352-70-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 785.40 | kJ/mol | NIST Webbook |
| basg | 756.00 | kJ/mol | NIST Webbook |
| gf | -83.97 | kJ/mol | Joback Method |
| hf | -158.86 | kJ/mol | Joback Method |
| hfus | 10.62 | kJ/mol | Joback Method |
| hvap | 33.30 | kJ/mol | Joback Method |
| ie | 8.92 ± 0.01 | eV | NIST Webbook |
| ie | 8.91 ± 0.01 | eV | NIST Webbook |
| log10ws | -2.28 | | Crippen Method |
| logp | 2.134 | | Crippen Method |
| mcvol | 87.500 | ml/mol | McGowan Method |
| pc | 3815.10 | kPa | Joback Method |
| rinpol | 761.60 | | NIST Webbook |
| rinpol | 756.00 | | NIST Webbook |
| rinpol | 778.00 | | NIST Webbook |
| rinpol | 774.00 | | NIST Webbook |
| rinpol | 778.00 | | NIST Webbook |
| rinpol | 769.00 | | NIST Webbook |
| rinpol | 769.00 | | NIST Webbook |
| rinpol | 783.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 769.00 | | NIST Webbook |
| tb | 389.50 ± 0.50 | K | NIST Webbook |
| tb | 389.20 | K | NIST Webbook |
| tc | 591.59 | K | Joback Method |
| tf | 162.35 ± 0.30 | K | NIST Webbook |
| tf | 184.00 ± 0.40 | K | NIST Webbook |
| vc | 0.338 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 147.93 | J/mol×K | 390.49 | Joback Method |
| cpg | 158.20 | J/mol×K | 424.01 | Joback Method |
| cpg | 167.93 | J/mol×K | 457.52 | Joback Method |
| cpg | 177.14 | J/mol×K | 491.04 | Joback Method |
| cpg | 185.85 | J/mol×K | 524.56 | Joback Method |
| cpg | 194.09 | J/mol×K | 558.07 | Joback Method |
| cpg | 201.85 | J/mol×K | 591.59 | Joback Method |
| hfust | 8.30 | kJ/mol | 183.95 | NIST Webbook |
| hfust | 8.30 | kJ/mol | 184.00 | NIST Webbook |
| hfust | 8.30 | kJ/mol | 184.00 | NIST Webbook |
| hfust | 6.31 | kJ/mol | 185.00 | NIST Webbook |
| hvapt | 41.60 | kJ/mol | 320.00 | NIST Webbook |
| hvapt | 39.20 | kJ/mol | 341.50 | NIST Webbook |
| hvapt | 40.70 | kJ/mol | 319.50 | NIST Webbook |
| sfust | 45.00 | J/mol×K | 183.95 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.43319e+01 |
| Coeff. B | -3.30694e+03 |
| Coeff. C | -4.90560e+01 |
| Temperature range (K), min. | 284.52 |
| Temperature range (K), max. | 415.66 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 4.94401e+00 |
| Coeff. B | -4.03266e+03 |
| Coeff. C | 1.72591e+00 |
| Coeff. D | -1.32384e-06 |
| Temperature range (K), min. | 308.15 |
| Temperature range (K), max. | 343.15 |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol1706.mol

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C352705&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**KDB Vapor Pressure Data:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1706

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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

**hfust:** Enthalpy of fusion at a given temperature

**hvap:** Enthalpy of vaporization at standard conditions

**hvapt:** Enthalpy of vaporization at a given temperature

**ie:** Ionization energy

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

| | |
|---|---|
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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