# 2,5-Difluorotoluene

**Other names:** Benzene, 1,4-difluoro-2-methyl-
**Inchi:** InChI=1S/C7H6F2/c1-5-4-6(8)2-3-7(5)9/h2-4H,1H3
**InchiKey:** YSNVKDGEALPJGC-UHFFFAOYSA-N
**Formula:** C7H6F2
**SMILES:** Cc1cc(F)ccc1F
**Mol. weight [g/mol]:** 128.12
**CAS:** 452-67-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -288.41 | kJ/mol | Joback Method |
| hf | -366.44 | kJ/mol | Joback Method |
| hfus | 13.31 | kJ/mol | Joback Method |
| hvap | 33.14 | kJ/mol | Joback Method |
| log10ws | -2.61 | | Crippen Method |
| logp | 2.273 | | Crippen Method |
| mcvol | 89.270 | ml/mol | McGowan Method |
| pc | 3547.31 | kPa | Joback Method |
| tb | 390.00 | K | NIST Webbook |
| tc | 586.20 | K | Joback Method |
| tf | 221.29 | K | Joback Method |
| vc | 0.355 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 157.53 | J/mol×K | 394.74 | Joback Method |
| cpg | 166.74 | J/mol×K | 426.65 | Joback Method |
| cpg | 175.52 | J/mol×K | 458.56 | Joback Method |
| cpg | 183.89 | J/mol×K | 490.47 | Joback Method |
| cpg | 191.84 | J/mol×K | 522.38 | Joback Method |
| cpg | 199.40 | J/mol×K | 554.29 | Joback Method |
| cpg | 206.58 | J/mol×K | 586.20 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 390.20 | K | 103.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47467e+01 |
| Coeff. B | -3.44786e+03 |
| Coeff. C | -4.95840e+01 |
| Temperature range (K), min. | 288.04 |
| Temperature range (K), max. | 415.01 |

# 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=C452675&Units=SI

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

**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 |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |