# 2,5-Dimethoxyfluorobenzene

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|---|---|
| **Other names:** | 1,4-Dimethoxy-2-fluorobenzene |
| | Benzene, 2-fluoro-1,4-dimethoxy- |
| **Inchi:** | InChI=1S/C8H9FO2/c1-10-6-3-4-8(11-2)7(9)5-6/h3-5H,1-2H3 |
| **InchiKey:** | WNCYZVMZKSOPMU-UHFFFAOYSA-N |
| **Formula:** | C8H9FO2 |
| **SMILES:** | COc1ccc(OC)c(F)c1 |
| **Mol. weight [g/mol]:** | 156.15 |
| **CAS:** | 82830-49-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -295.18 | kJ/mol | Joback Method |
| hf | -455.41 | kJ/mol | Joback Method |
| hfus | 15.20 | kJ/mol | Joback Method |
| hvap | 41.00 | kJ/mol | Joback Method |
| log10ws | -2.04 | | Crippen Method |
| logp | 1.843 | | Crippen Method |
| mcvol | 113.330 | ml/mol | McGowan Method |
| pc | 3213.68 | kPa | Joback Method |
| tb | 463.19 | K | Joback Method |
| tc | 661.91 | K | Joback Method |
| tf | 276.43 | K | Joback Method |
| vc | 0.429 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 229.97 | J/mol×K | 463.19 | Joback Method |
| cpg | 240.64 | J/mol×K | 496.31 | Joback Method |
| cpg | 250.93 | J/mol×K | 529.43 | Joback Method |
| cpg | 260.85 | J/mol×K | 562.55 | Joback Method |
| cpg | 270.37 | J/mol×K | 595.67 | Joback Method |
| cpg | 279.49 | J/mol×K | 628.79 | Joback Method |
| cpg | 288.21 | J/mol×K | 661.91 | Joback Method |

# Sources

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|---|---|
| **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=C82830497&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |