# Benzene, 1-fluoro-2-methoxy-

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|---|---|
| **Other names:** | 1-Fluoro-2-methoxybenzene |
| | 2-fluoroanisole |
| | 2-fluoromethoxybenzene |
| | anisole, o-fluoro- |
| | o-fluoroanisole |
| **Inchi:** | InChI=1S/C7H7FO/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3 |
| **InchiKey:** | JIXDOBAQOWOUPA-UHFFFAOYSA-N |
| **Formula:** | C7H7FO |
| **SMILES:** | COc1ccccc1F |
| **Mol. weight [g/mol]:** | 126.13 |
| **CAS:** | 321-28-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 808.00 | kJ/mol | NIST Webbook |
| basg | 778.00 | kJ/mol | NIST Webbook |
| gf | -188.97 | kJ/mol | Joback Method |
| hf | -291.08 | kJ/mol | Joback Method |
| hfus | 11.81 | kJ/mol | Joback Method |
| hvap | 52.10 ± 1.10 | kJ/mol | NIST Webbook |
| log10ws | -1.92 | | Crippen Method |
| logp | 1.834 | | Crippen Method |
| mcvol | 93.370 | ml/mol | McGowan Method |
| pc | 3736.23 | kPa | Joback Method |
| rinpol | 919.70 | | NIST Webbook |
| rinpol | 934.00 | | NIST Webbook |
| rinpol | 934.00 | | NIST Webbook |
| tb | 427.70 | K | NIST Webbook |
| tb | 427.50 ± 0.50 | K | NIST Webbook |
| tc | 613.45 | K | Joback Method |
| tf | 230.41 | K | Joback Method |
| vc | 0.355 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 169.33 | J/mol×K | 412.91 | Joback Method |
| cpg | 179.27 | J/mol×K | 446.33 | Joback Method |
| cpg | 188.77 | J/mol×K | 479.76 | Joback Method |
| cpg | 197.84 | J/mol×K | 513.18 | Joback Method |
| cpg | 206.49 | J/mol×K | 546.61 | Joback Method |
| cpg | 214.72 | J/mol×K | 580.03 | Joback Method |
| cpg | 222.53 | J/mol×K | 613.45 | Joback Method |
| hvapt | 52.20 | kJ/mol | 298.15 | Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers |

# 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=C321288&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Diffusion coefficients of 2-fluoroanisole, 2-bromoanisole, allylbenzene and 1,3-divinylbenzene at infinite dilution in supercritical carbon dioxide:** | https://www.doi.org/10.1016/j.fluid.2007.07.039 |
| **Experimental and computational study of the molecular energetics of the three monofluoroanisole isomers:** | https://www.doi.org/10.1016/j.jct.2008.09.012 |

# 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 |

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| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |