# 3-Fluorophenylacetic acid

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| **Other names:** | 3-Fluorophenlacetic acid |
| | m-Fluorophenylacetic acid |
| | Benzeneacetic acid, 3-fluoro- |
| | Acetic acid, (m-fluorophenyl)- |
| **Inchi:** | InChI=1S/C8H7FO2/c9-7-3-1-2-6(4-7)5-8(10)11/h1-4H,5H2,(H,10,11) |
| **InchiKey:** | YEAUYVGUXSZCFI-UHFFFAOYSA-N |
| **Formula:** | C8H7FO2 |
| **SMILES:** | O=C(O)Cc1cccc(F)c1 |
| **Mol. weight [g/mol]:** | 154.14 |
| **CAS:** | 331-25-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -341.29 | kJ/mol | Joback Method |
| hf | -444.31 | kJ/mol | Joback Method |
| hfus | 18.89 | kJ/mol | Joback Method |
| hvap | 58.95 | kJ/mol | Joback Method |
| log10ws | -1.70 | | Crippen Method |
| logp | 1.453 | | Crippen Method |
| mcvol | 109.030 | ml/mol | McGowan Method |
| pc | 4109.14 | kPa | Joback Method |
| tb | 559.42 | K | Joback Method |
| tc | 757.03 | K | Joback Method |
| tf | 330.20 | K | Joback Method |
| vc | 0.418 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 244.17 | J/mol×K | 559.42 | Joback Method |
| cpg | 253.02 | J/mol×K | 592.36 | Joback Method |
| cpg | 261.35 | J/mol×K | 625.29 | Joback Method |
| cpg | 269.17 | J/mol×K | 658.23 | Joback Method |
| cpg | 276.51 | J/mol×K | 691.16 | Joback Method |

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|---|---|---|---|---|
| cpg | 283.38 | J/mol×K | 724.10 | Joback Method |
| cpg | 289.80 | J/mol×K | 757.03 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=C331259&Units=SI |

# 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 |