

5-Fluoro-2-methylaniline

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|-----------------------------|--|
| Other names: | 2-Amino-4-fluorotoluene Benzenamine, 5-fluoro-2-methyl- 5-fluoro-o-toluidine |
| Inchi: | InChI=1S/C7H8FN/c1-5-2-3-6(8)4-7(5)9/h2-4H,9H2,1H3 |
| InchiKey: | JLCDTNLXUMYFQ-UHFFFAOYSA-N |
| Formula: | C7H8FN |
| SMILES: | Cc1ccc(F)cc1N |
| Mol. weight [g/mol]: | 125.14 |
| CAS: | 367-29-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -27.15 | kJ/mol | Joback Method |
| hf | -136.54 | kJ/mol | Joback Method |
| hfus | 15.43 | kJ/mol | Joback Method |
| hvap | 44.60 | kJ/mol | Joback Method |
| log10ws | -1.91 | | Crippen Method |
| logp | 1.716 | | Crippen Method |
| mcvol | 97.480 | ml/mol | McGowan Method |
| pc | 4021.02 | kPa | Joback Method |
| tb | 468.00 | K | Joback Method |
| tc | 685.00 | K | Joback Method |
| tf | 303.96 | K | Joback Method |
| vc | 0.366 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 196.53 | J/molxK | 468.00 | Joback Method |
| cpg | 206.84 | J/molxK | 504.17 | Joback Method |
| cpg | 216.58 | J/molxK | 540.33 | Joback Method |
| cpg | 225.78 | J/molxK | 576.50 | Joback Method |
| cpg | 234.45 | J/molxK | 612.66 | Joback Method |
| cpg | 242.60 | J/molxK | 648.83 | Joback Method |

cpg

250.26

J/mol×K

685.00

Joback Method

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 373.00 | K | 1.30 | NIST Webbook |

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=C367293&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307i |

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

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