

# (4-Fluorophenyl)acetone

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2-Propanone, 1-(4-fluorophenyl)-                         |
| <b>Inchi:</b>               | InChI=1S/C9H9FO/c1-7(11)6-8-2-4-9(10)5-3-8/h2-5H,6H2,1H3 |
| <b>InchiKey:</b>            | ZUEKIIWSVFBTCM-UHFFFAOYSA-N                              |
| <b>Formula:</b>             | C9H9FO   |
| <b>SMILES:</b>              | CC(=O)Cc1ccc(F)cc1                                       |
| <b>Mol. weight [g/mol]:</b> | 152.17   |
| <b>CAS:</b>                 | 459-03-0   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -196.05 | kJ/mol               | Joback Method  |
| hf            | -312.72 | kJ/mol               | Joback Method  |
| hfus          | 17.40   | kJ/mol               | Joback Method  |
| hvap          | 44.50   | kJ/mol               | Joback Method  |
| log10ws       | -2.30   |                      | Crippen Method |
| logp          | 1.957   |                      | Crippen Method |
| mcvol         | 117.250 | ml/mol               | McGowan Method |
| pc            | 3272.78 | kPa                  | Joback Method  |
| tb            | 490.12  | K                    | Joback Method  |
| tc            | 698.29  | K                    | Joback Method  |
| tf            | 280.65  | K                    | Joback Method  |
| vc            | 0.456   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 241.93 | J/mol×K | 490.12          | Joback Method |
| cpg           | 253.80 | J/mol×K | 524.82          | Joback Method |
| cpg           | 264.99 | J/mol×K | 559.51          | Joback Method |
| cpg           | 275.53 | J/mol×K | 594.21          | Joback Method |
| cpg           | 285.44 | J/mol×K | 628.90          | Joback Method |
| cpg           | 294.74 | J/mol×K | 663.60          | Joback Method |
| cpg           | 303.46 | J/mol×K | 698.29          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C459030&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C459030&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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