

Ethanone, 1-(2,4-difluorophenyl)-

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| Other names: | Acetophenone, 2',4'-difluoro- 2,4-Difluoroacetophenone 2',4'-Difluoroacetophenone 1-(2,4-difluorophenyl)ethan-1-one |
| Inchi: | InChI=1S/C8H6F2O/c1-5(11)7-3-2-6(9)4-8(7)10/h2-4H,1H3 |
| InchiKey: | QEWHNJPLPZOEKU-UHFFFAOYSA-N |
| Formula: | C8H6F2O |
| SMILES: | CC(=O)c1ccc(F)cc1F |
| Mol. weight [g/mol]: | 156.13 |
| CAS: | 364-83-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -408.91 | kJ/mol | Joback Method |
| hf | -499.66 | kJ/mol | Joback Method |
| hfus | 17.50 | kJ/mol | Joback Method |
| hvap | 42.11 | kJ/mol | Joback Method |
| log10ws | -2.79 | | Crippen Method |
| logp | 2.167 | | Crippen Method |
| mcvol | 104.930 | ml/mol | McGowan Method |
| pc | 3411.87 | kPa | Joback Method |
| tb | 471.49 | K | Joback Method |
| tc | 672.86 | K | Joback Method |
| tf | 282.49 | K | Joback Method |
| vc | 0.417 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 209.37 | J/molxK | 471.49 | Joback Method |
| cpg | 219.12 | J/molxK | 505.05 | Joback Method |
| cpg | 228.36 | J/molxK | 538.61 | Joback Method |
| cpg | 237.10 | J/molxK | 572.17 | Joback Method |
| cpg | 245.36 | J/molxK | 605.73 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 253.14 | J/mol×K | 639.29 | Joback Method |
| cpg | 260.45 | J/mol×K | 672.86 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|---------------|------|----------------|--------------|
| tbrp | 353.70 | K | 3.30 | NIST Webbook |
| tbrp | 353.50 ± 0.50 | K | 3.30 | 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=C364830&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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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