# Benzaldehyde, 4-fluoro-

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|---|---|
| **Other names:** | Benzaldehyde, p-fluoro-<br>p-Fluorobenzaldehyde<br>4-Fluorobenzaldehyde<br>para-Fluorobenzaldehyde |
| **Inchi:** | InChI=1S/C7H5FO/c8-7-3-1-6(5-9)2-4-7/h1-5H |
| **InchiKey:** | UOQXIWFBQSVDPP-UHFFFAOYSA-N |
| **Formula:** | C7H5FO |
| **SMILES:** | O=Cc1ccc(F)cc1 |
| **Mol. weight [g/mol]:** | 124.11 |
| **CAS:** | 459-57-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 827.10 | kJ/mol | NIST Webbook |
| basg | 795.30 | kJ/mol | NIST Webbook |
| ea | 0.49 ± 0.02 | eV | NIST Webbook |
| gf | -183.49 | kJ/mol | Joback Method |
| hf | -244.44 | kJ/mol | Joback Method |
| hfus | 12.91 | kJ/mol | Joback Method |
| hvap | 40.02 | kJ/mol | Joback Method |
| ie | 9.60 | eV | NIST Webbook |
| log10ws | -2.04 | | Crippen Method |
| logp | 1.638 | | Crippen Method |
| mcvol | 89.070 | ml/mol | McGowan Method |
| pc | 4189.32 | kPa | Joback Method |
| rinpol | 942.50 | | NIST Webbook |
| rinpol | 948.30 | | NIST Webbook |
| rinpol | 936.00 | | NIST Webbook |
| tb | 452.50 ± 0.50 | K | NIST Webbook |
| tc | 647.38 | K | Joback Method |
| tf | 250.18 | K | Joback Method |
| vc | 0.354 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 164.02 | J/mol×K | 439.15 | Joback Method |
| cpg | 173.14 | J/mol×K | 473.86 | Joback Method |
| cpg | 181.71 | J/mol×K | 508.56 | Joback Method |
| cpg | 189.77 | J/mol×K | 543.27 | Joback Method |
| cpg | 197.34 | J/mol×K | 577.97 | Joback Method |
| cpg | 204.42 | J/mol×K | 612.68 | Joback Method |
| cpg | 211.05 | J/mol×K | 647.38 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 454.20 | K | 101.00 | NIST Webbook |

# Sources

**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=C459574&Units=SI

# Legend

**affp:** Proton affinity
**basg:** Gas basicity
**cpg:** Ideal gas heat capacity
**ea:** Electron affinity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions

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|---|---|
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |