# 3,5-Difluorophenylacetic acid

**Inchi:** InChI=1S/C8H6F2O2/c9-6-1-5(3-8(11)12)2-7(10)4-6/h1-2,4H,3H2,(H,11,12)
**InchiKey:** IGGNSAVLXJKCNH-UHFFFAOYSA-N
**Formula:** C8H6F2O2
**SMILES:** O=C(O)Cc1cc(F)cc(F)c1
**Mol. weight [g/mol]:** 172.13
**CAS:** 105184-38-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -545.73 | kJ/mol | Joback Method |
| hf | -651.89 | kJ/mol | Joback Method |
| hfus | 21.59 | kJ/mol | Joback Method |
| hvap | 58.79 | kJ/mol | Joback Method |
| log10ws | -2.04 | | Crippen Method |
| logp | 1.592 | | Crippen Method |
| mcvol | 110.800 | ml/mol | McGowan Method |
| pc | 3810.39 | kPa | Joback Method |
| tb | 563.67 | K | Joback Method |
| tc | 753.30 | K | Joback Method |
| tf | 343.31 | K | Joback Method |
| vc | 0.436 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 251.48 | J/mol×K | 563.67 | Joback Method |
| cpg | 259.65 | J/mol×K | 595.28 | Joback Method |
| cpg | 267.37 | J/mol×K | 626.88 | Joback Method |
| cpg | 274.66 | J/mol×K | 658.49 | Joback Method |
| cpg | 281.52 | J/mol×K | 690.09 | Joback Method |
| cpg | 287.98 | J/mol×K | 721.70 | Joback Method |
| cpg | 294.04 | J/mol×K | 753.30 | Joback Method |

# 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=C105184381&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |