# 3-CF3-C6H4-CCH

**Inchi:** InChI=1S/C9H5F3/c1-2-7-4-3-5-8(6-7)9(10,11)12/h1,3-6H
**InchiKey:** PAHXLHWOHJTWRU-UHFFFAOYSA-N
**Formula:** C9H5F3
**SMILES:** C#Cc1cccc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 170.13
**CAS:** 705-28-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 806.20 | kJ/mol | NIST Webbook |
| basg | 773.80 | kJ/mol | NIST Webbook |
| gf | -230.84 | kJ/mol | Joback Method |
| hf | -309.21 | kJ/mol | Joback Method |
| hfus | 17.52 | kJ/mol | Joback Method |
| hvap | 34.68 | kJ/mol | Joback Method |
| log10ws | -3.27 | | Crippen Method |
| logp | 2.687 | | Crippen Method |
| mcvol | 110.620 | ml/mol | McGowan Method |
| pc | 3325.84 | kPa | Joback Method |
| tb | 421.68 | K | Joback Method |
| tc | 624.59 | K | Joback Method |
| tf | 281.29 | K | Joback Method |
| vc | 0.436 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 215.08 | J/mol×K | 421.68 | Joback Method |
| cpg | 226.50 | J/mol×K | 455.50 | Joback Method |
| cpg | 237.08 | J/mol×K | 489.32 | Joback Method |
| cpg | 246.87 | J/mol×K | 523.14 | Joback Method |
| cpg | 255.90 | J/mol×K | 556.95 | Joback Method |
| cpg | 264.24 | J/mol×K | 590.77 | Joback Method |
| cpg | 271.92 | J/mol×K | 624.59 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C705282&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |