# CF3C«equiv»CC«equiv»CCF3

**Other names:** 2,4-Hexadiyne, 1,1,1,6,6,6-hexafluoro-
2,4-Hexadiyne, hexafluoro-
Perfluorohexa-2,4-diyne
Hexafluoro-2,4-hexadiyne
Hexafluorohexa-2,4-diyne
**Inchi:** InChI=1S/C6F6/c7-5(8,9)3-1-2-4-6(10,11)12
**InchiKey:** IUMBVSOABSWHBN-UHFFFAOYSA-N
**Formula:** C6F6
**SMILES:** FC(F)(F)C#CC#CC(F)(F)F
**Mol. weight [g/mol]:** 186.05
**CAS:** 10524-09-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -757.94 | kJ/mol | Joback Method |
| hf | -816.73 | kJ/mol | Joback Method |
| hfus | 21.19 | kJ/mol | Joback Method |
| hvap | 25.76 | kJ/mol | Joback Method |
| ie | 11.50 ± 0.10 | eV | NIST Webbook |
| ie | 10.99 ± 0.01 | eV | NIST Webbook |
| log10ws | -3.25 | | Crippen Method |
| logp | 2.118 | | Crippen Method |
| mcvol | 88.820 | ml/mol | McGowan Method |
| pc | 3435.91 | kPa | Joback Method |
| tb | 343.84 | K | Joback Method |
| tc | 520.04 | K | Joback Method |
| tf | 377.96 | K | Joback Method |
| vc | 0.382 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 166.99 | J/mol×K | 343.84 | Joback Method |
| cpg | 174.93 | J/mol×K | 373.21 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 182.28 | J/mol×K | 402.57 | Joback Method |
| cpg | 189.07 | J/mol×K | 431.94 | Joback Method |
| cpg | 195.33 | J/mol×K | 461.31 | Joback Method |
| cpg | 201.09 | J/mol×K | 490.68 | Joback Method |
| cpg | 206.38 | J/mol×K | 520.04 | Joback Method |

# 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=C10524091&Units=SI

# 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
**ie:** Ionization energy
**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