# Butane, 1,1,2,3,4,4-hexachloro-tetrafluoro-

**Other names:** 1,1,2,3,4,4-Hexachloro-1,2,3,4-tetrafluorobutane
Butane, 1,1,2,3,4,4-hexachloro-tetrafluoro-
**Inchi:** InChI=1S/C4Cl6F4/c5-1(11,3(7,8)13)2(6,12)4(9,10)14
**InchiKey:** WWVUFVKMWDUDBV-UHFFFAOYSA-N
**Formula:** C4Cl6F4
**SMILES:** FC(Cl)(Cl)C(F)(Cl)C(F)(Cl)C(F)(Cl)Cl
**Mol. weight [g/mol]:** 336.75

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3390 | | Cheméo Relay (1.0) |
| gf | -856.66 | kJ/mol | Joback Method |
| hf | -1008.37 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 13.96 | kJ/mol | Joback Method |
| hvap | 52.22 | kJ/mol | Cheméo Relay (1.0) |
| ie | 11.18 | eV | Cheméo Relay (1.0) |
| log10ws | -5.68 | | Cheméo Relay (1.0) |
| logp | 4.997 | | Crippen Method |
| mcvol | 147.740 | ml/mol | McGowan Method |
| pc | 2690.21 | kPa | Joback Method |
| tb | 457.62 | K | Cheméo Relay (1.0) |
| tc | 671.07 | K | Cheméo Relay (1.0) |
| tf | 325.14 | K | Cheméo Relay (1.0) |
| vc | 0.547 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 273.30 | J/mol×K | 499.66 | Joback Method |
| cpg | 280.23 | J/mol×K | 536.12 | Joback Method |
| cpg | 286.03 | J/mol×K | 572.58 | Joback Method |
| cpg | 290.82 | J/mol×K | 609.04 | Joback Method |
| cpg | 294.70 | J/mol×K | 645.50 | Joback Method |
| cpg | 297.81 | J/mol×K | 681.96 | Joback Method |

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|---|---|---|---|---|
| cpg | 300.26 | J/mol×K | 718.43 | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C375439&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

# Legend

**af:** Acentric Factor
**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