# 1,5-Hexadien-3-ol, chlorodifluoroacetate

**Inchi:** InChI=1S/C8H9ClF2O2/c1-3-5-6(4-2)13-7(12)8(9,10)11/h3-4,6H,1-2,5H2
**InchiKey:** MNDIMJRVUZPCKP-UHFFFAOYSA-N
**Formula:** C8H9ClF2O2
**SMILES:** C=CCC(C=C)OC(=O)C(F)(F)Cl
**Mol. weight [g/mol]:** 210.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -442.91 | kJ/mol | Joback Method |
| hf | -624.38 | kJ/mol | Joback Method |
| hfus | 16.12 | kJ/mol | Joback Method |
| hvap | 42.28 | kJ/mol | Joback Method |
| log10ws | -2.82 | | Crippen Method |
| logp | 2.492 | | Crippen Method |
| mcvol | 138.200 | ml/mol | McGowan Method |
| pc | 2613.74 | kPa | Joback Method |
| rinpol | 920.00 | | NIST Webbook |
| tb | 484.39 | K | Joback Method |
| tc | 669.02 | K | Joback Method |
| tf | 267.08 | K | Joback Method |
| vc | 0.537 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 292.63 | J/mol×K | 484.39 | Joback Method |
| cpg | 303.37 | J/mol×K | 515.16 | Joback Method |
| cpg | 313.49 | J/mol×K | 545.93 | Joback Method |
| cpg | 323.01 | J/mol×K | 576.71 | Joback Method |
| cpg | 331.96 | J/mol×K | 607.48 | Joback Method |
| cpg | 340.36 | J/mol×K | 638.25 | Joback Method |
| cpg | 348.24 | J/mol×K | 669.02 | Joback Method |

# Sources

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|---|---|
| **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=U376230&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |