# 3-Hexanone, 2,2-dichloro

**Inchi:** InChI=1S/C6H10Cl2O/c1-3-4-5(9)6(2,7)8/h3-4H2,1-2H3
**InchiKey:** FFZAXGOQIDURKS-UHFFFAOYSA-N
**Formula:** C6H10Cl2O
**SMILES:** CCCC(=O)C(C)(Cl)Cl
**Mol. weight [g/mol]:** 169.05

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -150.30 | kJ/mol | Joback Method |
| hf | -319.98 | kJ/mol | Joback Method |
| hfus | 13.88 | kJ/mol | Joback Method |
| hvap | 43.17 | kJ/mol | Joback Method |
| log10ws | -2.53 | | Crippen Method |
| logp | 2.549 | | Crippen Method |
| mcvol | 121.450 | ml/mol | McGowan Method |
| pc | 3135.00 | kPa | Joback Method |
| rinpol | 957.00 | | NIST Webbook |
| rinpol | 957.00 | | NIST Webbook |
| tb | 462.18 | K | Joback Method |
| tc | 666.21 | K | Joback Method |
| tf | 269.57 | K | Joback Method |
| vc | 0.465 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 230.68 | J/mol×K | 462.18 | Joback Method |
| cpg | 241.10 | J/mol×K | 496.18 | Joback Method |
| cpg | 250.87 | J/mol×K | 530.19 | Joback Method |
| cpg | 260.00 | J/mol×K | 564.19 | Joback Method |
| cpg | 268.54 | J/mol×K | 598.20 | Joback Method |
| cpg | 276.51 | J/mol×K | 632.20 | Joback Method |
| cpg | 283.96 | J/mol×K | 666.21 | Joback Method |
| dvisc | 0.0052226 | Pa×s | 269.57 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0026645 | Pa×s | 301.67 | Joback Method |
| dvisc | 0.0015473 | Pa×s | 333.77 | Joback Method |
| dvisc | 0.0009885 | Pa×s | 365.88 | Joback Method |
| dvisc | 0.0006788 | Pa×s | 397.98 | Joback Method |
| dvisc | 0.0004930 | Pa×s | 430.08 | Joback Method |
| dvisc | 0.0003744 | Pa×s | 462.18 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R630172&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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |