# Hexachloroacetone

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|---|---|
| **Other names:** | 2-Propanone, 1,1,1,3,3,3-hexachloro- |
| | Bis(trichloromethyl) ketone |
| | Hexachloropropanone |
| | HCA |
| | Kureha HCA |
| | 1,1,1,3,3,3-Hexachloro-2-propanone |
| | 1,1,1,3,3,3-Hexachloropropanone |
| | 2-Propanone, hexachloro- |
| | Hexachloro-2-propanone |
| | Acetone, hexachloro- |
| | GC-1106 |
| | Perchloro-2-propanone |
| | HCA weedkiller |
| | UN 2661 |
| | NSC 6852 |
| | Perchloroacetone |
| **Inchi:** | InChI=1S/C3Cl6O/c4-2(5,6)1(10)3(7,8)9 |
| **InchiKey:** | DOJXGHGHTWFZHK-UHFFFAOYSA-N |
| **Formula:** | C3Cl6O |
| **SMILES:** | O=C(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl |
| **Mol. weight [g/mol]:** | 264.75 |
| **CAS:** | 116-16-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -220.44 | kJ/mol | Joback Method |
| hf | -329.77 | kJ/mol | Joback Method |
| hfus | 15.48 | kJ/mol | Joback Method |
| hvap | 52.74 | kJ/mol | Joback Method |
| log10ws | -3.48 | | Crippen Method |
| logp | 3.296 | | Crippen Method |
| mcvol | 128.140 | ml/mol | McGowan Method |
| pc | 3777.68 | kPa | Joback Method |
| rinpol | 1138.00 | | NIST Webbook |
| rinpol | 1138.00 | | NIST Webbook |
| tb | 476.20 | K | NIST Webbook |
| tc | 792.64 | K | Joback Method |

| | | | |
|---|---|---|---|
| tf | 357.86 | K | Joback Method |
| vc | 0.481 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 210.79 | J/mol×K | 750.54 | Joback Method |
| cpg | 204.50 | J/mol×K | 624.23 | Joback Method |
| cpg | 201.21 | J/mol×K | 582.13 | Joback Method |
| cpg | 197.15 | J/mol×K | 540.03 | Joback Method |
| cpg | 207.13 | J/mol×K | 666.33 | Joback Method |
| cpg | 212.00 | J/mol×K | 792.64 | Joback Method |
| cpg | 209.20 | J/mol×K | 708.43 | Joback Method |
| dvisc | 0.0034078 | Pa×s | 357.86 | Joback Method |
| dvisc | 0.0003726 | Pa×s | 540.03 | Joback Method |
| dvisc | 0.0004827 | Pa×s | 509.67 | Joback Method |
| dvisc | 0.0006463 | Pa×s | 479.31 | Joback Method |
| dvisc | 0.0009002 | Pa×s | 448.94 | Joback Method |
| dvisc | 0.0013155 | Pa×s | 418.58 | Joback Method |
| dvisc | 0.0020399 | Pa×s | 388.22 | Joback Method |
| hfust | 8.38 | kJ/mol | 147.70 | NIST Webbook |
| hvapt | 23.10 | kJ/mol | 229.00 | NIST Webbook |
| hvapt | 23.60 | kJ/mol | 220.50 | NIST Webbook |
| hvapt | 22.30 | kJ/mol | 298.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 341.20 | K | 0.80 | NIST Webbook |

# Sources

**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

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116165&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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