# .BETA.-chlordene

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|---|---|
| **Other names:** | 1,6-Methano-1H-indene, 2,3,3a,4,5,7-hexachloro-3a,6,7,7a-tetrahydro-, (1«alpha»,3a«beta»,6«alpha»,7«alpha»,7a«beta»)-<br>2,3,3a,4,5,7-Hexachloro-3a,6,7,7a-tetrahydro-1,6-methano-1H-indene-, (1«alpha»,3a«beta»,6«alpha»,7«alpha»,7a«beta»)-<br>1,6-Methano-1H-indene, 2,3,3a,4,5,7-hexachloro-3a,6,7,7a-tetrahydro-, (1R,3aR,6S,7S,7aR)-rel-<br>2,3,3a,4,5,7-Hexachloro-3a,6,7,7a-tetrahydro-1,6-methano-1H-indene |
| **Inchi:** | InChI=1S/C10H6Cl6/c11-5-3-1-2-4(5)10(16,8(14)6(2)12)9(15)7(3)13/h2-5H,1H2 |
| **InchiKey:** | OSFPUJNCRLXHDW-UHFFFAOYSA-N |
| **Formula:** | C10H6Cl6 |
| **SMILES:** | ClC1=C(Cl)C2(Cl)C(Cl)=C(Cl)C3CC1C(Cl)C32 |
| **Mol. weight [g/mol]:** | 338.88 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 35.88 | kJ/mol | Joback Method |
| logp | 5.229 | | Crippen Method |
| mcvol | 184.020 | ml/mol | McGowan Method |
| rinpol | 1925.80 | | NIST Webbook |
| rinpol | 1964.80 | | NIST Webbook |
| rinpol | 1898.00 | | NIST Webbook |
| rinpol | 1925.80 | | NIST Webbook |
| rinpol | 1898.00 | | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 395.62 | J/mol×K | 686.41 | Joback Method |
| cpg | 405.84 | J/mol×K | 729.32 | Joback Method |
| cpg | 415.64 | J/mol×K | 772.23 | Joback Method |
| cpg | 425.29 | J/mol×K | 815.14 | Joback Method |
| cpg | 435.06 | J/mol×K | 858.05 | Joback Method |
| cpg | 445.23 | J/mol×K | 900.96 | Joback Method |
| cpg | 456.08 | J/mol×K | 943.87 | Joback Method |

# Sources

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|---|---|
| **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):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C56534033&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |