

# 1,6-Methano-1H-indene, 2,3,3a,4,5,8-hexachloro-3a,6,7,7a-tetrahydro-, (1-«alpha»,3a-«beta»,6-«alpha»,7a-«beta»,8R\*)-

Other names:

«gamma»-Chlordene

Inchi: InChI=1S/C10H6Cl6/c11-5-2-1-3-4(5)7(13)9(15)10(3,16)8(14)6(2)12/h2-5H,1H2

InchiKey: SVGYVZYRIHEIML-UHFFFAOYSA-N

Formula: C10H6Cl6

SMILES: ClC1=C(Cl)C2(Cl)C(Cl)=C(Cl)C3C(Cl)C1CC32

Mol. weight [g/mol]: 338.87

CAS: 56641-38-4

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 132.38  | kJ/mol               | Joback Method  |
| hf            | -87.69  | kJ/mol               | Joback Method  |
| hfus          | 35.88   | kJ/mol               | Joback Method  |
| hvap          | 65.54   | kJ/mol               | Joback Method  |
| log10ws       | -5.80   |                      | Crippen Method |
| logp          | 5.229   |                      | Crippen Method |
| mcvol         | 184.020 | ml/mol               | McGowan Method |
| pc            | 2515.07 | kPa                  | Joback Method  |
| rinpol        | 1902.00 |                      | NIST Webbook   |
| rinpol        | 1917.40 |                      | NIST Webbook   |
| rinpol        | 1959.60 |                      | NIST Webbook   |
| ripol         | 2628.00 |                      | NIST Webbook   |
| ripol         | 2628.00 |                      | NIST Webbook   |
| tb            | 686.41  | K                    | Joback Method  |
| tc            | 943.87  | K                    | Joback Method  |
| tf            | 499.30  | K                    | Joback Method  |
| vc            | 0.721   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 395.62 | J/molxK | 686.41          | Joback Method |
| cpg           | 405.84 | J/molxK | 729.32          | Joback Method |
| cpg           | 415.64 | J/molxK | 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

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C56641384&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56641384&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>   |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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