

# 4,7-Methano-1H-indene, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-

|                      |                                                                                                                                                                                                                                                           |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 4,5,6,7,8,8-Hexachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene<br>4,7-Methanoindene, 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-<br>4,7-Methanoindene, 4,5,6,7,8,8-hexachloro-«delta»<br>4,7-Methanoindene, 4,5,6,7,8,8-hexachloro-Â«deltaÂ»<br>Chlordene |
| Inchi:               | InChI=1S/C10H6Cl6/c11-6-7(12)9(14)5-3-1-2-4(5)8(6,13)10(9,15)16/h1-2,4-5H,3H2                                                                                                                                                                             |
| InchiKey:            | XCJXQCUJXDUNDN-UHFFFAOYSA-N                                                                                                                                                                                                                               |
| Formula:             | C10H6Cl6                                                                                                                                                                                                                                                  |
| SMILES:              | C1C1=C(Cl)C2(Cl)C3CC=CC3C1(Cl)C2(Cl)Cl                                                                                                                                                                                                                    |
| Mol. weight [g/mol]: | 338.87                                                                                                                                                                                                                                                    |
| CAS:                 | 3734-48-3                                                                                                                                                                                                                                                 |

## Physical Properties

| Property code | Value   | Unit    | Source                      |
|---------------|---------|---------|-----------------------------|
| gf            | 140.66  | kJ/mol  | Joback Method               |
| hf            | -34.27  | kJ/mol  | Joback Method               |
| hfus          | 24.06   | kJ/mol  | Joback Method               |
| hvap          | 61.91   | kJ/mol  | Joback Method               |
| log10ws       | -5.64   |         | Estimated Solubility Method |
| logp          | 5.024   |         | Crippen Method              |
| mcvol         | 184.020 | ml/mol  | McGowan Method              |
| pc            | 2847.48 | kPa     | Joback Method               |
| rinpol        | 1755.40 |         | NIST Webbook                |
| rinpol        | 1755.40 |         | NIST Webbook                |
| rinpol        | 1778.30 |         | NIST Webbook                |
| tb            | 676.93  | K       | Joback Method               |
| tc            | 954.03  | K       | Joback Method               |
| tf            | 522.06  | K       | Joback Method               |
| vc            | 0.717   | m3/kmol | Joback Method               |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 391.21 | J/mol×K | 676.93 | Joback Method |
| cpg | 401.11 | J/mol×K | 723.11 | Joback Method |
| cpg | 411.33 | J/mol×K | 769.30 | Joback Method |
| cpg | 422.59 | J/mol×K | 815.48 | Joback Method |
| cpg | 435.62 | J/mol×K | 861.66 | Joback Method |
| cpg | 451.15 | J/mol×K | 907.84 | Joback Method |
| cpg | 469.90 | J/mol×K | 954.03 | Joback Method |

## Sources

|                                     |                                                                                                                                                                                                   |
|-------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Joback Method:</b>               | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                             |
| <b>Estimated Solubility Method:</b> | <a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a> |
| <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=C3734483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3734483&amp;Units=SI</a>                                                       |
| <b>Crippen Method:</b>              | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>mccvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-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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