

# 2-endo,3-exo,5-endo,6-exo,8b,9c,10a-heptachloro

**Inchi:** InChI=1S/C10H11Cl7/c11-1-9(2-12)4-5(14)7(16)10(9,3-13)8(17)6(4)15/h4-8H,1-3H2/t4?,  
**InchiKey:** LQZCWWYZXXZBKE-UUNWVVFUSA-N  
**Formula:** C10H11Cl7  
**SMILES:** ClC1(CCl)C2C(Cl)C(Cl)C1(CCl)C(Cl)C2Cl  
**Mol. weight [g/mol]:** 379.37

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 9.68    | kJ/mol               | Joback Method  |
| hf            | -291.69 | kJ/mol               | Joback Method  |
| hfus          | 37.96   | kJ/mol               | Joback Method  |
| hvap          | 64.70   | kJ/mol               | Joback Method  |
| log10ws       | -4.59   |                      | Crippen Method |
| logp          | 4.749   |                      | Crippen Method |
| mvol          | 215.720 | ml/mol               | McGowan Method |
| pc            | 2016.32 | kPa                  | Joback Method  |
| rmpol         | 2190.20 |                      | NIST Webbook   |
| tb            | 685.09  | K                    | Joback Method  |
| tc            | 929.85  | K                    | Joback Method  |
| tf            | 470.86  | K                    | Joback Method  |
| vc            | 0.836   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 492.98 | J/mol×K | 685.09          | Joback Method |
| cpg           | 506.36 | J/mol×K | 725.88          | Joback Method |
| cpg           | 519.36 | J/mol×K | 766.68          | Joback Method |
| cpg           | 532.30 | J/mol×K | 807.47          | Joback Method |
| cpg           | 545.50 | J/mol×K | 848.26          | Joback Method |
| cpg           | 559.29 | J/mol×K | 889.06          | Joback Method |
| cpg           | 573.99 | J/mol×K | 929.85          | 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=R502537&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R502537&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>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>h vap:</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>m cvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>r inpol:</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                                 |

Latest version available from:

<https://www.chemeo.com/cid/30-189-9/2-endo-3-exo-5-endo-6-exo-8b-9c-10a-heptachlorobornane.pdf>

Generated by Cheméo on 2024-04-19 01:53:52.064123053 +0000 UTC m=+15780880.984700366.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.