

# NAPHTHALENE, 1,2,3,6,7,8-HEXACHLORO-

**Inchi:** InChI=1S/C10H2Cl6/c11-4-1-3-2-5(12)8(14)10(16)6(3)9(15)7(4)13/h1-2H  
**InchiKey:** WJYZNPLWZGYFIE-UHFFFAOYSA-N  
**Formula:** C10H2Cl6  
**SMILES:** Clc1cc2cc(Cl)c(Cl)c(Cl)c2c(Cl)c1Cl  
**Mol. weight [g/mol]:** 334.84

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | 35.08   | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 35.56   | kJ/mol | Joback Method      |
| hvap          | 93.89   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.40    | eV     | Cheméo Relay (1.0) |
| log10ws       | -8.23   |        | Cheméo Relay (1.0) |
| logp          | 6.760   |        | Crippen Method     |
| mcvol         | 181.980 | ml/mol | McGowan Method     |
| rinpol        | 2505.00 |        | NIST Webbook       |
| rinpol        | 2505.00 |        | NIST Webbook       |
| rinpol        | 2505.00 |        | NIST Webbook       |
| tb            | 637.40  | K      | Cheméo Relay (1.0) |
| tf            | 466.14  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 325.21    | J/mol×K | 728.32          | Joback Method |
| cpg           | 331.53    | J/mol×K | 772.43          | Joback Method |
| cpg           | 337.34    | J/mol×K | 816.54          | Joback Method |
| cpg           | 342.69    | J/mol×K | 860.66          | Joback Method |
| cpg           | 347.65    | J/mol×K | 904.77          | Joback Method |
| cpg           | 352.28    | J/mol×K | 948.88          | Joback Method |
| cpg           | 356.64    | J/mol×K | 992.99          | Joback Method |
| dvisc         | 0.0008492 | Pa×s    | 516.22          | Joback Method |
| dvisc         | 0.0006870 | Pa×s    | 551.57          | Joback Method |
| dvisc         | 0.0005701 | Pa×s    | 586.92          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004832 | Pa×s | 622.27 | Joback Method |
| dvisc | 0.0004169 | Pa×s | 657.62 | Joback Method |
| dvisc | 0.0003651 | Pa×s | 692.97 | Joback Method |
| dvisc | 0.0003240 | Pa×s | 728.32 | 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>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17062872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17062872&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>ie:</b>      | Ionization energy                               |
| <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>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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