

# Naphthalene, 1,2,4,6,8-pentachloro

|                             |                                                                         |
|-----------------------------|-------------------------------------------------------------------------|
| <b>Other names:</b>         | 1,2,4,6,8-pentachloronaphthalene<br>naphthalene, 1,2,4,6,8-pentachloro- |
| <b>Inchi:</b>               | InChI=1S/C10H3Cl5/c11-4-1-5-6(12)3-8(14)10(15)9(5)7(13)2-4/h1-3H        |
| <b>InchiKey:</b>            | HGSDQSUMXKHGTH-UHFFFAOYSA-N                                             |
| <b>Formula:</b>             | C10H3Cl5                                                                |
| <b>SMILES:</b>              | Clc1cc(Cl)c2c(Cl)c(Cl)cc(Cl)c2c1                                        |
| <b>Mol. weight [g/mol]:</b> | 300.40                                                                  |

## Physical Properties

| Property code | Value   | Unit                 | Source                                                                                            |
|---------------|---------|----------------------|---------------------------------------------------------------------------------------------------|
| gf            | 144.58  | kJ/mol               | Joback Method                                                                                     |
| hf            | 41.82   | kJ/mol               | Joback Method                                                                                     |
| hfus          | 19.75   | kJ/mol               | Evaluation of entropies of fusion of polychlorinated naphthalenes by model congeners: A DSC study |
| hvap          | 67.00   | kJ/mol               | Joback Method                                                                                     |
| log10ws       | -6.70   |                      | Crippen Method                                                                                    |
| logp          | 6.107   |                      | Crippen Method                                                                                    |
| mcvol         | 169.740 | ml/mol               | McGowan Method                                                                                    |
| pc            | 2884.30 | kPa                  | Joback Method                                                                                     |
| rinpol        | 2178.00 |                      | NIST Webbook                                                                                      |
| rinpol        | 2178.00 |                      | NIST Webbook                                                                                      |
| tb            | 685.91  | K                    | Joback Method                                                                                     |
| tc            | 947.92  | K                    | Joback Method                                                                                     |
| tf            | 473.78  | K                    | Joback Method                                                                                     |
| vc            | 0.654   | m <sup>3</sup> /kmol | Joback Method                                                                                     |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 310.73 | J/mol×K | 685.91          | Joback Method |
| cpg           | 341.68 | J/mol×K | 904.25          | Joback Method |
| cpg           | 336.44 | J/mol×K | 860.58          | Joback Method |
| cpg           | 330.79 | J/mol×K | 816.91          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 324.67    | J/molxK | 773.25 | Joback Method |
| cpg   | 318.01    | J/molxK | 729.58 | Joback Method |
| cpg   | 346.58    | J/molxK | 947.92 | Joback Method |
| dvisc | 0.0003445 | Paxs    | 685.91 | Joback Method |
| dvisc | 0.0003907 | Paxs    | 650.56 | Joback Method |
| dvisc | 0.0004495 | Paxs    | 615.20 | Joback Method |
| dvisc | 0.0005262 | Paxs    | 579.85 | Joback Method |
| dvisc | 0.0006286 | Paxs    | 544.49 | Joback Method |
| dvisc | 0.0007697 | Paxs    | 509.14 | Joback Method |
| dvisc | 0.0009715 | Paxs    | 473.78 | Joback Method |

## Sources

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Evaluation of entropies of fusion of polychlorinated naphthalenes by model Joback Method DSC study:**

<https://www.doi.org/10.1016/j.tca.2006.04.011>

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R128664&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>mccol:</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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