

# 2,2',3,3',4,5',6-Heptachlorobiphenyl

|                      |                                                                                                      |
|----------------------|------------------------------------------------------------------------------------------------------|
| Other names:         | 2,2',3,3',4,5',6-Heptachloro-1,1'-biphenyl<br>1,1'-Biphenyl, 2,2',3,3',4,5',6-heptachloro<br>PCB 175 |
| Inchi:               | InChI=1S/C12H3Cl7/c13-4-1-5(10(17)7(15)2-4)9-6(14)3-8(16)11(18)12(9)19/h1-3H                         |
| InchiKey:            | KJBDZJFSYQUNJT-UHFFFAOYSA-N                                                                          |
| Formula:             | C12H3Cl7                                                                                             |
| SMILES:              | Clc1cc(Cl)c(Cl)c(-c2c(Cl)cc(Cl)c(Cl)c2Cl)c1                                                          |
| Mol. weight [g/mol]: | 395.32                                                                                               |
| CAS:                 | 40186-70-7                                                                                           |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 124.06  | kJ/mol  | Joback Method  |
| hf            | -8.42   | kJ/mol  | Joback Method  |
| hfus          | 41.57   | kJ/mol  | Joback Method  |
| hvap          | 82.19   | kJ/mol  | Joback Method  |
| log10ws       | -8.87   |         | Crippen Method |
| logp          | 7.927   |         | Crippen Method |
| mcvol         | 218.100 | ml/mol  | McGowan Method |
| pc            | 2329.27 | kPa     | Joback Method  |
| rinpol        | 2387.00 |         | NIST Webbook   |
| rinpol        | 2387.00 |         | NIST Webbook   |
| tb            | 824.19  | K       | Joback Method  |
| tc            | 1096.84 | K       | Joback Method  |
| tf            | 574.92  | K       | Joback Method  |
| vc            | 0.835   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 415.14 | J/mol×K | 824.19          | Joback Method |
| cpg           | 422.07 | J/mol×K | 869.63          | Joback Method |
| cpg           | 428.26 | J/mol×K | 915.07          | Joback Method |
| cpg           | 433.75 | J/mol×K | 960.51          | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 438.58    | J/mol×K | 1005.96 | Joback Method |
| cpg   | 442.79    | J/mol×K | 1051.40 | Joback Method |
| cpg   | 446.42    | J/mol×K | 1096.84 | Joback Method |
| dvisc | 0.0004373 | Pa×s    | 574.92  | Joback Method |
| dvisc | 0.0003321 | Pa×s    | 616.47  | Joback Method |
| dvisc | 0.0002611 | Pa×s    | 658.01  | Joback Method |
| dvisc | 0.0002113 | Pa×s    | 699.56  | Joback Method |
| dvisc | 0.0001750 | Pa×s    | 741.10  | Joback Method |
| dvisc | 0.0001479 | Pa×s    | 782.64  | Joback Method |
| dvisc | 0.0001272 | Pa×s    | 824.19  | 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=C40186707&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40186707&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>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>mcvol:</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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