

# Chloroform, deuterio-

**Inchi:** InChI=1S/CHCl3/c2-1(3)4/h1H/i1D  
**InchiKey:** HEDRZPFGACZZDS-MICDWDOJSA-N  
**Formula:** CHCl3  
**SMILES:** [2H]C(Cl)(Cl)Cl  
**Mol. weight [g/mol]:** 120.38

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.1169  |         | Cheméo Relay (1.0) |
| gf            | -80.69  | kJ/mol  | Joback Method      |
| hf            | -160.23 | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 7.41    | kJ/mol  | Joback Method      |
| hvap          | 26.90   | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 11.31   | eV      | Cheméo Relay (1.0) |
| log10ws       | -2.12   |         | Cheméo Relay (1.0) |
| logp          | 1.986   |         | Crippen Method     |
| mcvol         | 61.670  | ml/mol  | McGowan Method     |
| pc            | 4980.35 | kPa     | Joback Method      |
| tb            | 304.75  | K       | Cheméo Relay (1.0) |
| tc            | 577.16  | K       | Cheméo Relay (1.0) |
| tf            | 215.06  | K       | Cheméo Relay (1.0) |
| vc            | 0.260   | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 71.18     | J/mol×K | 334.13          | Joback Method |
| cpg           | 73.44     | J/mol×K | 367.13          | Joback Method |
| cpg           | 75.56     | J/mol×K | 400.12          | Joback Method |
| cpg           | 77.54     | J/mol×K | 433.12          | Joback Method |
| cpg           | 79.40     | J/mol×K | 466.12          | Joback Method |
| cpg           | 81.13     | J/mol×K | 499.12          | Joback Method |
| cpg           | 82.74     | J/mol×K | 532.11          | Joback Method |
| dvisc         | 0.0053758 | Pa×s    | 175.79          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0026426 | Pa×s | 202.18 | Joback Method |
| dvisc | 0.0015306 | Pa×s | 228.57 | Joback Method |
| dvisc | 0.0009926 | Pa×s | 254.96 | Joback Method |
| dvisc | 0.0006982 | Pa×s | 281.35 | Joback Method |
| dvisc | 0.0005216 | Pa×s | 307.74 | Joback Method |
| dvisc | 0.0004081 | Pa×s | 334.13 | Joback Method |

## Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007499&Units=SI>

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>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <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>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>pc:</b>      | Critical Pressure                               |
| <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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