

# Methane, dibromochloro-

|                      |                               |
|----------------------|-------------------------------|
| Other names:         | CDBM                          |
|                      | CHClBr <sub>2</sub>           |
|                      | Chlorobromoform               |
|                      | Chlorodibromomethane          |
|                      | Chlorodibromomethane          |
|                      | Dibromochloromethane          |
|                      | Dibromomono-chloromethane     |
|                      | Methane, chlorodibromo-       |
|                      | Mono-chlorodibromomethane     |
|                      | NCI-C55254                    |
| Inchi:               | InChI=1S/CHBr2Cl/c2-1(3)4/h1H |
| InchiKey:            | GATVIKZLVQHOMN-UHFFFAOYSA-N   |
| Formula:             | CHBr <sub>2</sub> Cl          |
| SMILES:              | ClC(Br)Br                     |
| Mol. weight [g/mol]: | 208.28                        |
| CAS:                 | 124-48-1                      |

## Physical Properties

| Property code | Value        | Unit   | Source                               |
|---------------|--------------|--------|--------------------------------------|
| gf            | -28.19       | kJ/mol | Joback Method                        |
| hf            | -32.33       | kJ/mol | Joback Method                        |
| hfus          | 9.59         | kJ/mol | Joback Method                        |
| hvap          | 34.69        | kJ/mol | Joback Method                        |
| ie            | 10.69        | eV     | NIST Webbook                         |
| ie            | 10.59 ± 0.01 | eV     | NIST Webbook                         |
| ie            | 10.50        | eV     | NIST Webbook                         |
| ie            | 10.59 ± 0.01 | eV     | NIST Webbook                         |
| log10ws       | -1.90        |        | Aqueous Solubility Prediction Method |
| log10ws       | -1.90        |        | Estimated Solubility Method          |
| logp          | 2.299        |        | Crippen Method                       |
| mccvol        | 72.190       | ml/mol | McGowan Method                       |
| pc            | 6886.93      | kPa    | Joback Method                        |
| rinpol        | 776.00       |        | NIST Webbook                         |
| rinpol        | 776.00       |        | NIST Webbook                         |

|        |         |         |                                      |
|--------|---------|---------|--------------------------------------|
| rinpol | 768.00  |         | NIST Webbook                         |
| rinpol | 768.00  |         | NIST Webbook                         |
| rinpol | 768.00  |         | NIST Webbook                         |
| rinpol | 818.00  |         | NIST Webbook                         |
| rinpol | 783.00  |         | NIST Webbook                         |
| rinpol | 759.00  |         | NIST Webbook                         |
| rinpol | 783.00  |         | NIST Webbook                         |
| rinpol | 792.00  |         | NIST Webbook                         |
| rinpol | 775.00  |         | NIST Webbook                         |
| rinpol | 766.50  |         | NIST Webbook                         |
| rinpol | 800.00  |         | NIST Webbook                         |
| rinpol | 764.00  |         | NIST Webbook                         |
| rinpol | 800.00  |         | NIST Webbook                         |
| rinpol | 809.00  |         | NIST Webbook                         |
| rinpol | 770.00  |         | NIST Webbook                         |
| ripol  | 1310.00 |         | NIST Webbook                         |
| ripol  | 1267.00 |         | NIST Webbook                         |
| ripol  | 1267.00 |         | NIST Webbook                         |
| ripol  | 1304.75 |         | NIST Webbook                         |
| ripol  | 1322.01 |         | NIST Webbook                         |
| ripol  | 1316.36 |         | NIST Webbook                         |
| tb     | 391.59  | K       | Joback Method                        |
| tc     | 618.86  | K       | Joback Method                        |
| tf     | 251.82  | K       | Aqueous Solubility Prediction Method |
| vc     | 0.259   | m3/kmol | Joback Method                        |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 77.59     | J/mol×K | 391.59          | Joback Method |
| cpg           | 80.06     | J/mol×K | 429.47          | Joback Method |
| cpg           | 82.26     | J/mol×K | 467.35          | Joback Method |
| cpg           | 84.20     | J/mol×K | 505.22          | Joback Method |
| cpg           | 85.91     | J/mol×K | 543.10          | Joback Method |
| cpg           | 87.42     | J/mol×K | 580.98          | Joback Method |
| cpg           | 88.75     | J/mol×K | 618.86          | Joback Method |
| dvisc         | 0.0039165 | Pa×s    | 235.55          | Joback Method |
| dvisc         | 0.0023767 | Pa×s    | 261.56          | Joback Method |
| dvisc         | 0.0015786 | Pa×s    | 287.56          | Joback Method |
| dvisc         | 0.0011222 | Pa×s    | 313.57          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008405 | Pa×s | 339.58 | Joback Method |
| dvisc | 0.0006560 | Pa×s | 365.58 | Joback Method |
| dvisc | 0.0005291 | Pa×s | 391.59 | Joback Method |

## Sources

|                                                                                               |                                                                                                                                                                                                                         |
|-----------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>                                                                          | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C124481&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C124481&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>Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:</b> | <a href="https://www.doi.org/10.1021/je3010535">https://www.doi.org/10.1021/je3010535</a>                                                                                                                               |
| <b>Joback Method</b>                                                                          | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                                                   |
| <b>Aqueous Solubility Prediction Method:</b>                                                  | <a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a> |
| <b>Estimated Solubility Method:</b>                                                           | <a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>                       |
| <b>McGowan Method:</b>                                                                        | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>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>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | 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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