

# 1-bromo-2-chloropropane

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C3H6BrCl/c1-3(5)2-4/h3H,2H2,1H3 |
| <b>InchiKey:</b>            | YMHXXJJTAGKFBA-UHFFFAOYSA-N              |
| <b>Formula:</b>             | C3H6BrCl                                 |
| <b>SMILES:</b>              | CC(Cl)CBr                                |
| <b>Mol. weight [g/mol]:</b> | 157.44                                   |
| <b>CAS:</b>                 | 3017-96-7                                |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -25.67  | kJ/mol  | Joback Method  |
| hf            | -99.94  | kJ/mol  | Joback Method  |
| hfus          | 9.48    | kJ/mol  | Joback Method  |
| hvap          | 32.70   | kJ/mol  | Joback Method  |
| log10ws       | -1.77   |         | Crippen Method |
| logp          | 2.009   |         | Crippen Method |
| mcvol         | 82.870  | ml/mol  | McGowan Method |
| pc            | 4652.99 | kPa     | Joback Method  |
| tb            | 391.00  | K       | NIST Webbook   |
| tc            | 571.70  | K       | Joback Method  |
| tf            | 198.29  | K       | Joback Method  |
| vc            | 0.308   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 116.80    | J/molxK | 371.19          | Joback Method |
| cpg           | 123.09    | J/molxK | 404.61          | Joback Method |
| cpg           | 129.03    | J/molxK | 438.03          | Joback Method |
| cpg           | 134.65    | J/molxK | 471.44          | Joback Method |
| cpg           | 139.96    | J/molxK | 504.86          | Joback Method |
| cpg           | 144.97    | J/molxK | 538.28          | Joback Method |
| cpg           | 149.70    | J/molxK | 571.70          | Joback Method |
| dvisc         | 0.0052743 | Paxs    | 198.29          | Joback Method |
| dvisc         | 0.0026310 | Paxs    | 227.11          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0015350 | Paxs | 255.92 | Joback Method |
| dvisc | 0.0009987 | Paxs | 284.74 | Joback Method |
| dvisc | 0.0007032 | Paxs | 313.56 | Joback Method |
| dvisc | 0.0005253 | Paxs | 342.37 | Joback Method |
| dvisc | 0.0004106 | Paxs | 371.19 | 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=C3017967&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3017967&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>mccvol:</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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