# 1-Bromo-1-chloroethane

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|---|---|
| **Other names:** | CH3CHClBr |
| | Ethane, 1-bromo-1-chloro- |
| **Inchi:** | InChI=1S/C2H4BrCl/c1-2(3)4/h2H,1H3 |
| **InchiKey:** | QMSVNDSDEZTYAS-UHFFFAOYSA-N |
| **Formula:** | C2H4BrCl |
| **SMILES:** | CC(Cl)Br |
| **Mol. weight [g/mol]:** | 143.41 |
| **CAS:** | 593-96-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -34.09 | kJ/mol | Joback Method |
| hf | -81.00 ± 3.00 | kJ/mol | NIST Webbook |
| hfus | 6.90 | kJ/mol | Joback Method |
| hvap | 30.48 | kJ/mol | Joback Method |
| ie | 10.37 | eV | NIST Webbook |
| ie | 10.42 | eV | NIST Webbook |
| log10ws | -1.85 | | Crippen Method |
| logp | 1.966 | | Crippen Method |
| mcvol | 68.780 | ml/mol | McGowan Method |
| pc | 5327.93 | kPa | Joback Method |
| tb | 356.20 | K | NIST Webbook |
| tc | 549.86 | K | Joback Method |
| tf | 187.02 | K | Joback Method |
| vc | 0.253 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 86.20 | J/mol×K | 348.31 | Joback Method |
| cpg | 90.75 | J/mol×K | 381.90 | Joback Method |
| cpg | 95.03 | J/mol×K | 415.49 | Joback Method |
| cpg | 99.07 | J/mol×K | 449.09 | Joback Method |
| cpg | 102.86 | J/mol×K | 482.68 | Joback Method |

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|---|---|---|---|---|
| cpg | 106.43 | J/mol×K | 516.27 | Joback Method |
| cpg | 109.79 | J/mol×K | 549.86 | Joback Method |
| dvisc | 0.0025302 | Pa×s | 213.90 | Joback Method |
| dvisc | 0.0049301 | Pa×s | 187.02 | Joback Method |
| dvisc | 0.0015071 | Pa×s | 240.78 | Joback Method |
| dvisc | 0.0009961 | Pa×s | 267.66 | Joback Method |
| dvisc | 0.0007101 | Pa×s | 294.55 | Joback Method |
| dvisc | 0.0005357 | Pa×s | 321.43 | Joback Method |
| dvisc | 0.0004221 | Pa×s | 348.31 | Joback Method |
| hvapt | 33.10 | kJ/mol | 323.00 | NIST Webbook |
| hvapt | 46.70 | kJ/mol | 296.50 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 354.10 ± 0.50 | K | 98.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.18014e+01 |
| Coeff. B | -1.77343e+03 |
| Coeff. C | -1.09259e+02 |
| Temperature range (K), min. | 263.29 |
| Temperature range (K), max. | 382.52 |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**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=C593964&Units=SI

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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