# Ethane, 1-bromo-2-chloro-

| | |
|---|---|
| **Other names:** | 1,2-Bromochloroethane |
| | 1,2-Chlorobromoethane |
| | 1-Bromo-2-chloroethane |
| | 1-Chloro-2-bromoethane |
| | 1-bromo-2-chloroethyne |
| | 2-Bromo-1-chloroethane |
| | 2-Bromoethyl chloride |
| | 2-Chloroethyl bromide |
| | CH2BrCH2Cl |
| | Ethylene chlorobromide |
| | NSC 60186 |
| | s-Chlorobromoethane |
| | sym-Chlorobromoethane |
| | «beta»-Chloroethyl bromide |
| | Â«betaÂ»-Chloroethyl bromide |
| **Inchi:** | InChI=1S/C2H4BrCl/c3-1-2-4/h1-2H2 |
| **InchiKey:** | IBYHHJPAARCAIE-UHFFFAOYSA-N |
| **Formula:** | C2H4BrCl |
| **SMILES:** | ClCCBr |
| **Mol. weight [g/mol]:** | 143.41 |
| **CAS:** | 107-04-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -31.65 | kJ/mol | Joback Method |
| hf | -74.02 | kJ/mol | Joback Method |
| hfus | 10.42 | kJ/mol | Joback Method |
| hvap | 38.13 ± 0.04 | kJ/mol | NIST Webbook |
| ie | 10.55 | eV | NIST Webbook |
| ie | 10.63 ± 0.03 | eV | NIST Webbook |
| ie | 10.50 ± 0.10 | eV | NIST Webbook |
| ie | 10.70 ± 0.10 | eV | NIST Webbook |
| ie | 10.65 ± 0.01 | eV | NIST Webbook |
| ie | 10.52 | eV | NIST Webbook |
| ie | 10.57 ± 0.05 | eV | NIST Webbook |
| ie | 10.63 | eV | NIST Webbook |

| | | | |
|---|---|---|---|
| log10ws | -1.32 | | Aqueous Solubility Prediction Method |
| log10ws | -1.32 | | Estimated Solubility Method |
| logp | 1.620 | | Crippen Method |
| mcvol | 68.780 | ml/mol | McGowan Method |
| pc | 5266.25 | kPa | Joback Method |
| rinpol | 704.00 | | NIST Webbook |
| rinpol | 723.00 | | NIST Webbook |
| rinpol | 716.00 | | NIST Webbook |
| rinpol | 725.20 | | NIST Webbook |
| rinpol | 688.00 | | NIST Webbook |
| rinpol | 693.00 | | NIST Webbook |
| rinpol | 698.00 | | NIST Webbook |
| rinpol | 729.00 | | NIST Webbook |
| rinpol | 681.00 | | NIST Webbook |
| rinpol | 708.00 | | NIST Webbook |
| ripol | 1174.97 | | NIST Webbook |
| ripol | 1186.26 | | NIST Webbook |
| ripol | 1186.26 | | NIST Webbook |
| ripol | 1192.67 | | NIST Webbook |
| tb | 348.75 | K | Joback Method |
| tc | 545.22 | K | Joback Method |
| tf | 256.40 | K | NIST Webbook |
| tf | 198.80 ± 0.40 | K | NIST Webbook |
| tf | 256.50 ± 0.20 | K | NIST Webbook |
| tf | 255.92 | K | Aqueous Solubility Prediction Method |
| vc | 0.259 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 86.29 | J/mol×K | 348.75 | Joback Method |
| cpg | 94.69 | J/mol×K | 414.24 | Joback Method |
| cpg | 98.54 | J/mol×K | 446.99 | Joback Method |
| cpg | 102.17 | J/mol×K | 479.73 | Joback Method |
| cpg | 105.59 | J/mol×K | 512.48 | Joback Method |
| cpg | 108.82 | J/mol×K | 545.22 | Joback Method |
| cpg | 90.61 | J/mol×K | 381.50 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpl | 136.77 | J/mol×K | 295.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.84 | J/mol×K | 297.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.89 | J/mol×K | 298.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.92 | J/mol×K | 298.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.99 | J/mol×K | 300.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 137.07 | J/mol×K | 301.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.15 | J/mol×K | 303.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.23 | J/mol×K | 304.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.31 | J/mol×K | 306.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.39 | J/mol×K | 307.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 137.48 | J/mol×K | 309.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.57 | J/mol×K | 310.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.66 | J/mol×K | 312.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.75 | J/mol×K | 313.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 137.84 | J/mol×K | 315.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 137.93 | J/mol×K | 316.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.03 | J/mol×K | 318.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.13 | J/mol×K | 319.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.22 | J/mol×K | 321.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.33 | J/mol×K | 322.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 138.43 | J/mol×K | 324.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.53 | J/mol×K | 325.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.64 | J/mol×K | 327.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.74 | J/mol×K | 328.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 138.85 | J/mol×K | 330.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 138.96 | J/mol×K | 331.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 139.07 | J/mol×K | 333.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 139.19 | J/mol×K | 334.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 139.30 | J/mol×K | 336.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 139.42 | J/mol×K | 337.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 139.54 | J/mol×K | 339.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 139.66 | J/mol×K | 340.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 139.78 | J/mol×K | 342.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 139.90 | J/mol×K | 343.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 140.03 | J/mol×K | 345.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 140.16 | J/mol×K | 346.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 140.29 | J/mol×K | 348.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 140.42 | J/mol×K | 349.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 140.55 | J/mol×K | 351.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 140.68 | J/mol×K | 352.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 140.82 | J/mol×K | 354.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.70 | J/mol×K | 294.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 130.10 | J/mol×K | 300.00 | NIST Webbook |
| cpl | 136.63 | J/mol×K | 292.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.56 | J/mol×K | 291.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.50 | J/mol×K | 289.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |

| | | | | |
|---|---|---|---|---|
| cpl | 136.43 | J/mol×K | 288.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.37 | J/mol×K | 286.65 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 140.91 | J/mol×K | 355.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| cpl | 136.31 | J/mol×K | 285.15 | Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K |
| dvisc | 0.0004315 | Pa×s | 348.75 | Joback Method |
| dvisc | 0.0005304 | Pa×s | 324.30 | Joback Method |
| dvisc | 0.0031520 | Pa×s | 202.02 | Joback Method |
| dvisc | 0.0018920 | Pa×s | 226.48 | Joback Method |
| dvisc | 0.0012545 | Pa×s | 250.93 | Joback Method |
| dvisc | 0.0008948 | Pa×s | 275.38 | Joback Method |
| dvisc | 0.0006744 | Pa×s | 299.84 | Joback Method |
| hfust | 3.10 | kJ/mol | 182.00 | NIST Webbook |
| hfust | 9.62 | kJ/mol | 256.40 | NIST Webbook |
| hfust | 9.62 | kJ/mol | 256.40 | NIST Webbook |
| hvapt | 39.50 | kJ/mol | 311.50 | NIST Webbook |
| hvapt | 36.40 ± 0.10 | kJ/mol | 338.00 | NIST Webbook |
| hvapt | 36.60 ± 0.10 | kJ/mol | 330.00 | NIST Webbook |
| hvapt | 36.90 ± 0.10 | kJ/mol | 323.00 | NIST Webbook |

| | | | | |
|---|---|---|---|---|
| hvapt | 37.30 ± 0.10 | kJ/mol | 315.00 | NIST Webbook |
| hvapt | 38.06 | kJ/mol | 379.80 | NIST Webbook |
| hvapt | 37.60 ± 0.10 | kJ/mol | 308.00 | NIST Webbook |
| pvap | 8.91 | kPa | 313.15 | Isothermal Vapor-Liquid Equilibria of ethyl acetate + dibromomethane, or + bromochloromethane or + 1,2-dichloroethane or +1-bromo-2-chloroethane at T = 313.15 K |
| rhol | 1727.01 | kg/m3 | 298.15 | (Vapor + liquid) equilibria for the binary mixtures (1-propanol + dibromomethane, or + bromochloromethane, or + 1,2-dichloroethane or +1-bromo-2-chloroethane) at T = 313.15 K. |
| sfust | 37.53 | J/mol×K | 256.40 | NIST Webbook |
| sfust | 17.15 | J/mol×K | 182.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.31363e+01 |
| Coeff. B | -2.60209e+03 |
| Coeff. C | -7.46670e+01 |
| Temperature range (K), min. | 272.75 |
| Temperature range (K), max. | 407.21 |

# Sources

| | |
|---|---|
| **Temperature and Pressure Dependence of the Volumetric Properties of Binary Liquid Mixtures Containing Dihaloalkanes:** | https://www.doi.org/10.1007/s10765-005-5570-x |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C107040&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Heat Capacity of alpha,omega-Bromochloroalkanes and Their Dependence on the Hydrocarbon Chain Length and Temperature (288.15 to 353.15) K:** | https://www.doi.org/10.1021/je201002j |
| **(Vapour + liquid) equilibria for the binary mixtures (1-propanol + 1,1-dibromoethane or + bromochloromethane, or + 1,2-dichloroethane or +1-bromo-2-chloroethane) at T = 313.15 K:** | https://www.doi.org/10.1016/j.jct.2004.07.012 |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Isothermal Vapor-Liquid Equilibria of ethyl acetate + dibromomethane, or + bromochloromethane or + 1,2-dichloroethane or +1-bromo-2-chloroethane at T = 313.15 K:** | https://www.doi.org/10.1021/je034259j |
| **Joback Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |