# Ethane, 1,1-dibromo-

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|---|---|
| **Other names:** | 1,1-Dibromoethane |
| | CH3CHBr2 |
| | Dibromoethane |
| | ETHYLIDENE DIBROMIDE |
| | Ethylidene bromide |
| **Inchi:** | InChI=1S/C2H4Br2/c1-2(3)4/h2H,1H3 |
| **InchiKey:** | APQIUTYORBAGEZ-UHFFFAOYSA-N |
| **Formula:** | C2H4Br2 |
| **SMILES:** | CC(Br)Br |
| **Mol. weight [g/mol]:** | 187.86 |
| **CAS:** | 557-91-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -7.84 | kJ/mol | Joback Method |
| hf | -41.00 | kJ/mol | NIST Webbook |
| hfus | 7.98 | kJ/mol | Joback Method |
| hvap | 32.53 | kJ/mol | Joback Method |
| ie | 10.19 ± 0.03 | eV | NIST Webbook |
| ie | 10.17 | eV | NIST Webbook |
| ie | 10.17 | eV | NIST Webbook |
| log10ws | -2.13 | | Crippen Method |
| logp | 2.122 | | Crippen Method |
| mcvol | 74.040 | ml/mol | McGowan Method |
| pc | 6259.01 | kPa | Joback Method |
| rinpol | 712.00 | | NIST Webbook |
| rinpol | 718.00 | | NIST Webbook |
| rinpol | 698.00 | | NIST Webbook |
| rinpol | 706.00 | | NIST Webbook |
| rinpol | 724.00 | | NIST Webbook |
| tb | 382.65 ± 0.70 | K | NIST Webbook |
| tb | 381.20 | K | NIST Webbook |
| tc | 592.98 | K | Joback Method |
| tf | 216.90 | K | Joback Method |
| vc | 0.266 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 91.34 | J/mol×K | 377.04 | Joback Method |
| cpg | 111.78 | J/mol×K | 556.99 | Joback Method |
| cpg | 108.28 | J/mol×K | 521.00 | Joback Method |
| cpg | 104.51 | J/mol×K | 485.01 | Joback Method |
| cpg | 100.45 | J/mol×K | 449.02 | Joback Method |
| cpg | 96.07 | J/mol×K | 413.03 | Joback Method |
| cpg | 115.02 | J/mol×K | 592.98 | Joback Method |
| dvisc | 0.0004806 | Pa×s | 377.04 | Joback Method |
| dvisc | 0.0006009 | Pa×s | 350.35 | Joback Method |
| dvisc | 0.0007796 | Pa×s | 323.66 | Joback Method |
| dvisc | 0.0010599 | Pa×s | 296.97 | Joback Method |
| dvisc | 0.0015312 | Pa×s | 270.28 | Joback Method |
| dvisc | 0.0023976 | Pa×s | 243.59 | Joback Method |
| dvisc | 0.0041922 | Pa×s | 216.90 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.40647e+01 |
| Coeff. B | -3.06198e+03 |
| Coeff. C | -5.70550e+01 |
| Temperature range (K), min. | 279.31 |
| Temperature range (K), max. | 406.87 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 5.57186e+01 |
| Coeff. B | -6.50116e+03 |
| Coeff. C | -5.75296e+00 |
| Coeff. D | 1.01867e-06 |
| Temperature range (K), min. | 210.15 |

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|---|---|
| Temperature range (K), max. | 628.00 |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1570.mol |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C557915&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1570 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |