# 1,1,1,2-Tetrabromoethane

**Other names:** Ethane, 1,1,1,2-tetrabromo-
**Inchi:** InChI=1S/C2H2Br4/c3-1-2(4,5)6/h1H2
**InchiKey:** RVHSTXJKKZWWDQ-UHFFFAOYSA-N
**Formula:** C2H2Br4
**SMILES:** BrCC(Br)(Br)Br
**Mol. weight [g/mol]:** 345.65
**CAS:** 630-16-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 26.08 | kJ/mol | Joback Method |
| hf | 11.96 | kJ/mol | Joback Method |
| hfus | 14.66 | kJ/mol | Joback Method |
| hvap | 44.49 | kJ/mol | Joback Method |
| log10ws | -3.49 | | Crippen Method |
| logp | 3.220 | | Crippen Method |
| mcvol | 109.040 | ml/mol | McGowan Method |
| pc | 8043.60 | kPa | Joback Method |
| tb | 506.57 | K | Joback Method |
| tc | 774.77 | K | Joback Method |
| tf | 353.92 | K | Joback Method |
| vc | 0.385 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 152.51 | J/mol×K | 774.77 | Joback Method |
| cpg | 138.19 | J/mol×K | 506.57 | Joback Method |
| cpg | 141.95 | J/mol×K | 551.27 | Joback Method |
| cpg | 145.01 | J/mol×K | 595.97 | Joback Method |
| cpg | 147.47 | J/mol×K | 640.67 | Joback Method |
| cpg | 149.46 | J/mol×K | 685.37 | Joback Method |
| cpg | 151.10 | J/mol×K | 730.07 | Joback Method |
| dvisc | 0.0004563 | Pa×s | 506.57 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0022584 | Pa×s | 353.92 | Joback Method |
| dvisc | 0.0015821 | Pa×s | 379.36 | Joback Method |
| dvisc | 0.0011590 | Pa×s | 404.80 | Joback Method |
| dvisc | 0.0008808 | Pa×s | 430.25 | Joback Method |
| dvisc | 0.0006903 | Pa×s | 455.69 | Joback Method |
| dvisc | 0.0005551 | Pa×s | 481.13 | Joback Method |
| hvapt | 61.50 | kJ/mol | 402.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.72925e+01 |
| Coeff. B | -5.30440e+03 |
| Coeff. C | -8.65860e+01 |
| Temperature range (K), min. | 398.52 |
| Temperature range (K), max. | 529.32 |

# Sources

**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=C630160&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |