# 1-Propene, 1-bromo-

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|---|---|
| **Other names:** | 1-Bromo-1-propene |
| | 1-Bromopropene |
| | 1-Bromopropylene |
| | 1-Propenyl bromide |
| | Propene, 1-bromo- |
| | Propenyl bromide |
| **Inchi:** | InChI=1S/C3H5Br/c1-2-3-4/h2-3H,1H3 |
| **InchiKey:** | NNQDMQVWOWCVEM-UHFFFAOYSA-N |
| **Formula:** | C3H5Br |
| **SMILES:** | CC=CBr |
| **Mol. weight [g/mol]:** | 120.98 |
| **CAS:** | 590-14-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 68.92 | kJ/mol | Joback Method |
| hf | 38.30 | kJ/mol | Joback Method |
| hfus | 9.01 | kJ/mol | Joback Method |
| hvap | 28.67 | kJ/mol | Joback Method |
| ie | 9.30 ± 0.05 | eV | NIST Webbook |
| log10ws | -1.86 | | Crippen Method |
| logp | 1.915 | | Crippen Method |
| mcvol | 66.330 | ml/mol | McGowan Method |
| pc | 5213.15 | kPa | Joback Method |
| tb | 333.70 | K | NIST Webbook |
| tc | 534.95 | K | Joback Method |
| tf | 178.29 | K | Joback Method |
| vc | 0.245 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 107.57 | J/mol×K | 502.18 | Joback Method |
| cpg | 103.12 | J/mol×K | 469.42 | Joback Method |

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|---|---|---|---|---|
| cpg | 98.35 | J/mol×K | 436.65 | Joback Method |
| cpg | 93.25 | J/mol×K | 403.89 | Joback Method |
| cpg | 87.80 | J/mol×K | 371.12 | Joback Method |
| cpg | 81.97 | J/mol×K | 338.36 | Joback Method |
| cpg | 111.73 | J/mol×K | 534.95 | Joback Method |
| dvisc | 0.0028576 | Pa×s | 178.29 | Joback Method |
| dvisc | 0.0002964 | Pa×s | 338.36 | Joback Method |
| dvisc | 0.0003679 | Pa×s | 311.68 | Joback Method |
| dvisc | 0.0004755 | Pa×s | 285.00 | Joback Method |
| dvisc | 0.0006479 | Pa×s | 258.32 | Joback Method |
| dvisc | 0.0009481 | Pa×s | 231.65 | Joback Method |
| dvisc | 0.0015320 | Pa×s | 204.97 | Joback Method |
| hvapt | 32.00 | kJ/mol | 311.50 | NIST Webbook |
| hvapt | 32.50 | kJ/mol | 317.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52488e+01 |
| Coeff. B | -3.18697e+03 |
| Coeff. C | -3.39050e+01 |
| Temperature range (K), min. | 246.92 |
| Temperature range (K), max. | 354.61 |

# 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=C590147&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 |
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |