# Benzene, 1-bromo-2-ethyl-

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|---|---|
| **Other names:** | 1-Bromo-2-ethylbenzene |
| | 1-Ethyl-2-bromobenzene |
| | 2-Bromo-1-ethylbenzene |
| | 2-Ethylbromobenzene |
| | o-Bromoethylbenzene |
| **Inchi:** | InChI=1S/C8H9Br/c1-2-7-5-3-4-6-8(7)9/h3-6H,2H2,1H3 |
| **InchiKey:** | HVRUGFJYCAFAAN-UHFFFAOYSA-N |
| **Formula:** | C8H9Br |
| **SMILES:** | CCc1ccccc1Br |
| **Mol. weight [g/mol]:** | 185.06 |
| **CAS:** | 1973-22-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 133.58 | kJ/mol | Joback Method |
| hf | 42.94 | kJ/mol | Joback Method |
| hfus | 15.41 | kJ/mol | Joback Method |
| hvap | 42.78 | kJ/mol | Joback Method |
| log10ws | -3.44 | | Crippen Method |
| logp | 3.012 | | Crippen Method |
| mcvol | 117.320 | ml/mol | McGowan Method |
| pc | 3901.37 | kPa | Joback Method |
| rinpol | 1166.00 | | NIST Webbook |
| rinpol | 1166.00 | | NIST Webbook |
| tb | 472.50 | K | NIST Webbook |
| tb | 474.65 ± 0.07 | K | NIST Webbook |
| tc | 710.10 | K | Joback Method |
| tf | 205.61 ± 0.05 | K | NIST Webbook |
| tf | 205.90 ± 0.70 | K | NIST Webbook |
| vc | 0.438 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 272.56 | J/mol×K | 710.10 | Joback Method |
| cpg | 264.29 | J/mol×K | 671.79 | Joback Method |
| cpg | 255.40 | J/mol×K | 633.48 | Joback Method |
| cpg | 245.87 | J/mol×K | 595.18 | Joback Method |
| cpg | 235.65 | J/mol×K | 556.87 | Joback Method |
| cpg | 224.69 | J/mol×K | 518.57 | Joback Method |
| cpg | 212.97 | J/mol×K | 480.26 | Joback Method |
| dvisc | 0.0021418 | Pa×s | 278.66 | Joback Method |
| dvisc | 0.0002886 | Pa×s | 480.26 | Joback Method |
| dvisc | 0.0003554 | Pa×s | 446.66 | Joback Method |
| dvisc | 0.0004529 | Pa×s | 413.06 | Joback Method |
| dvisc | 0.0006024 | Pa×s | 379.46 | Joback Method |
| dvisc | 0.0008469 | Pa×s | 345.86 | Joback Method |
| dvisc | 0.0012813 | Pa×s | 312.26 | Joback Method |
| hvapt | 48.10 | kJ/mol | 445.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.40866e+01 |
| Coeff. B | -3.78741e+03 |
| Coeff. C | -7.24910e+01 |
| Temperature range (K), min. | 346.96 |
| Temperature range (K), max. | 504.10 |

# 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=C1973224&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |