# Benzene, (bromoethynyl)-

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|---|---|
| **Other names:** | (Bromoethynyl)benzene |
| | Bromophenylacetylene |
| | Phenylethynyl bromide |
| | 1-Bromo-2-phenylacetylene |
| | 1-Phenyl-2-bromoacetylene |
| **Inchi:** | InChI=1S/C8H5Br/c9-7-6-8-4-2-1-3-5-8/h1-5H |
| **InchiKey:** | BPVHWNVBBDHIQU-UHFFFAOYSA-N |
| **Formula:** | C8H5Br |
| **SMILES:** | BrC#Cc1ccccc1 |
| **Mol. weight [g/mol]:** | 181.03 |
| **CAS:** | 932-87-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 346.01 | kJ/mol | Joback Method |
| hf | 326.71 | kJ/mol | Joback Method |
| hfus | 18.92 | kJ/mol | Joback Method |
| hvap | 44.27 | kJ/mol | Joback Method |
| ie | 8.65 | eV | NIST Webbook |
| log10ws | -3.10 | | Crippen Method |
| logp | 2.390 | | Crippen Method |
| mcvol | 108.720 | ml/mol | McGowan Method |
| pc | 4917.69 | kPa | Joback Method |
| tb | 484.28 | K | Joback Method |
| tc | 746.44 | K | Joback Method |
| tf | 372.24 | K | Joback Method |
| vc | 0.400 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 180.08 | J/mol×K | 484.28 | Joback Method |
| cpg | 190.59 | J/mol×K | 527.97 | Joback Method |
| cpg | 200.23 | J/mol×K | 571.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 209.06 | J/mol×K | 615.36 | Joback Method |
| cpg | 217.15 | J/mol×K | 659.05 | Joback Method |
| cpg | 224.55 | J/mol×K | 702.74 | Joback Method |
| cpg | 231.33 | J/mol×K | 746.44 | Joback Method |

# Sources

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|---|---|
| **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=C932876&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |