# Benzene, 1,3-butadienyl-

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|---|---|
| **Other names:** | 1,3-Butadiene, 1-phenyl- |
| | 1-Phenylbutadiene |
| | 1-Phenyl-1,3-butadiene |
| | 1,3-Butadienylbenzene |
| **Inchi:** | InChI=1S/C10H10/c1-2-3-7-10-8-5-4-6-9-10/h2-9H,1H2 |
| **InchiKey:** | XZKRXPZXQLARHH-UHFFFAOYSA-N |
| **Formula:** | C10H10 |
| **SMILES:** | C=CC=Cc1ccccc1 |
| **Mol. weight [g/mol]:** | 130.19 |
| **CAS:** | 1515-78-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 313.79 | kJ/mol | Joback Method |
| hf | 229.45 | kJ/mol | Joback Method |
| hfus | 14.62 | kJ/mol | Joback Method |
| hvap | 39.42 | kJ/mol | Joback Method |
| ie | 8.39 | eV | NIST Webbook |
| log10ws | -2.99 | | Crippen Method |
| logp | 2.886 | | Crippen Method |
| mcvol | 119.400 | ml/mol | McGowan Method |
| pc | 3254.14 | kPa | Joback Method |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 177.00 | | NIST Webbook |
| ripol | 1572.00 | | NIST Webbook |
| tb | 455.72 | K | Joback Method |
| tc | 675.61 | K | Joback Method |
| tf | 222.04 | K | Joback Method |
| vc | 0.449 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 223.50 | J/mol×K | 455.72 | Joback Method |

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|---|---|---|---|---|
| cpg | 237.60 | J/mol×K | 492.37 | Joback Method |
| cpg | 250.71 | J/mol×K | 529.02 | Joback Method |
| cpg | 262.90 | J/mol×K | 565.67 | Joback Method |
| cpg | 274.22 | J/mol×K | 602.32 | Joback Method |
| cpg | 284.74 | J/mol×K | 638.97 | Joback Method |
| cpg | 294.51 | J/mol×K | 675.61 | Joback Method |
| dvisc | 0.0030060 | Pa×s | 222.04 | Joback Method |
| dvisc | 0.0013450 | Pa×s | 260.99 | Joback Method |
| dvisc | 0.0007416 | Pa×s | 299.93 | Joback Method |
| dvisc | 0.0004689 | Pa×s | 338.88 | Joback Method |
| dvisc | 0.0003258 | Pa×s | 377.83 | Joback Method |
| dvisc | 0.0002424 | Pa×s | 416.77 | Joback Method |
| dvisc | 0.0001896 | Pa×s | 455.72 | Joback Method |

# Sources

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|---|---|
| **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=C1515782&Units=SI |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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https://www.chemeo.com/cid/67-775-8/Benzene-1-3-butadienyl.pdf

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