# Bicyclo[2.2.2]octane, 2-chloro-

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|---|---|
| **Other names:** | 2-Chlorobicyclo[2.2.2]octane |
| **Inchi:** | InChI=1S/C8H13Cl/c9-8-5-6-1-3-7(8)4-2-6/h6-8H,1-5H2 |
| **InchiKey:** | PTVXDQZENDCNDA-UHFFFAOYSA-N |
| **Formula:** | C8H13Cl |
| **SMILES:** | ClC1CC2CCC1CC2 |
| **Mol. weight [g/mol]:** | 144.64 |
| **CAS:** | 33649-79-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 94.14 | kJ/mol | Joback Method |
| hf | -111.25 | kJ/mol | Joback Method |
| hfus | 13.81 | kJ/mol | Joback Method |
| hvap | 37.65 | kJ/mol | Joback Method |
| log10ws | -2.74 | | Crippen Method |
| logp | 2.804 | | Crippen Method |
| mcvol | 114.100 | ml/mol | McGowan Method |
| pc | 3280.28 | kPa | Joback Method |
| tb | 437.22 | K | Joback Method |
| tc | 654.25 | K | Joback Method |
| tf | 234.44 | K | Joback Method |
| vc | 0.429 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 231.23 | J/mol×K | 437.22 | Joback Method |
| cpg | 249.10 | J/mol×K | 473.39 | Joback Method |
| cpg | 265.84 | J/mol×K | 509.56 | Joback Method |
| cpg | 281.49 | J/mol×K | 545.74 | Joback Method |
| cpg | 296.12 | J/mol×K | 581.91 | Joback Method |
| cpg | 309.79 | J/mol×K | 618.08 | Joback Method |
| cpg | 322.55 | J/mol×K | 654.25 | Joback Method |
| dvisc | 0.0012972 | Pa×s | 234.44 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0010562 | Pa×s | 268.24 | Joback Method |
| dvisc | 0.0009005 | Pa×s | 302.03 | Joback Method |
| dvisc | 0.0007927 | Pa×s | 335.83 | Joback Method |
| dvisc | 0.0007144 | Pa×s | 369.63 | Joback Method |
| dvisc | 0.0006550 | Pa×s | 403.42 | Joback Method |
| dvisc | 0.0006088 | Pa×s | 437.22 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=C33649795&Units=SI |

# 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 |
| **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 |

Latest version available from:
https://www.chemeo.com/cid/67-387-9/Bicyclo-2-2-2-octane-2-chloro.pdf
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