# Benzene, (1-chloropropyl)

**Inchi:** InChI=1S/C9H11Cl/c1-2-9(10)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3
**InchiKey:** MZMVVHAHSRJOEO-UHFFFAOYSA-N
**Formula:** C9H11Cl
**SMILES:** CCC(Cl)c1ccccc1
**Mol. weight [g/mol]:** 154.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 122.94 | kJ/mol | Joback Method |
| hf | -13.58 | kJ/mol | Joback Method |
| hfus | 13.78 | kJ/mol | Joback Method |
| hvap | 41.90 | kJ/mol | Joback Method |
| log10ws | -3.30 | | Crippen Method |
| logp | 3.377 | | Crippen Method |
| mcvol | 126.150 | ml/mol | McGowan Method |
| pc | 3156.17 | kPa | Joback Method |
| rinpol | 1133.00 | | NIST Webbook |
| rinpol | 1131.00 | | NIST Webbook |
| tb | 468.99 | K | Joback Method |
| tc | 687.77 | K | Joback Method |
| tf | 232.53 | K | Joback Method |
| vc | 0.474 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 242.63 | J/mol×K | 468.99 | Joback Method |
| cpg | 256.41 | J/mol×K | 505.45 | Joback Method |
| cpg | 269.33 | J/mol×K | 541.92 | Joback Method |
| cpg | 281.43 | J/mol×K | 578.38 | Joback Method |
| cpg | 292.74 | J/mol×K | 614.85 | Joback Method |
| cpg | 303.30 | J/mol×K | 651.31 | Joback Method |
| cpg | 313.15 | J/mol×K | 687.77 | Joback Method |
| dvisc | 0.0050859 | Pa×s | 232.53 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0021248 | Pa×s | 271.94 | Joback Method |
| dvisc | 0.0011072 | Pa×s | 311.35 | Joback Method |
| dvisc | 0.0006679 | Pa×s | 350.76 | Joback Method |
| dvisc | 0.0004463 | Pa×s | 390.17 | Joback Method |
| dvisc | 0.0003211 | Pa×s | 429.58 | Joback Method |
| dvisc | 0.0002441 | Pa×s | 468.99 | 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=R129632&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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |