# Benzene, 1-methyl-4-(1-chloro-1-methylethyl)

**Inchi:** InChI=1S/C10H13Cl/c1-8-4-6-9(7-5-8)10(2,3)11/h4-7H,1-3H3
**InchiKey:** ITTZHNHXCRWVKL-UHFFFAOYSA-N
**Formula:** C10H13Cl
**SMILES:** Cc1ccc(C(C)(C)Cl)cc1
**Mol. weight [g/mol]:** 168.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 127.01 | kJ/mol | Joback Method |
| hf | -49.16 | kJ/mol | Joback Method |
| hfus | 12.09 | kJ/mol | Joback Method |
| hvap | 43.88 | kJ/mol | Joback Method |
| log10ws | -3.49 | | Crippen Method |
| logp | 3.469 | | Crippen Method |
| mcvol | 140.240 | ml/mol | McGowan Method |
| pc | 2829.33 | kPa | Joback Method |
| tb | 494.06 | K | Joback Method |
| tc | 720.15 | K | Joback Method |
| tf | 273.74 | K | Joback Method |
| vc | 0.525 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 288.69 | J/mol×K | 494.06 | Joback Method |
| cpg | 303.90 | J/mol×K | 531.74 | Joback Method |
| cpg | 318.04 | J/mol×K | 569.42 | Joback Method |
| cpg | 331.18 | J/mol×K | 607.10 | Joback Method |
| cpg | 343.37 | J/mol×K | 644.79 | Joback Method |
| cpg | 354.69 | J/mol×K | 682.47 | Joback Method |
| cpg | 365.18 | J/mol×K | 720.15 | Joback Method |
| dvisc | 0.0033165 | Pa×s | 273.74 | Joback Method |
| dvisc | 0.0016285 | Pa×s | 310.46 | Joback Method |
| dvisc | 0.0009295 | Pa×s | 347.18 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005906 | Pa×s | 383.90 | Joback Method |
| dvisc | 0.0004062 | Pa×s | 420.62 | Joback Method |
| dvisc | 0.0002967 | Pa×s | 457.34 | Joback Method |
| dvisc | 0.0002270 | Pa×s | 494.06 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R131878&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |