# 2-Chloro-4-iodotoluene

**Other names:** Benzene, 2-chloro-4-iodo-1-methyl-
**Inchi:** InChI=1S/C7H6ClI/c1-5-2-3-6(9)4-7(5)8/h2-4H,1H3
**InchiKey:** PJYASWQMTNNSSL-UHFFFAOYSA-N
**Formula:** C7H6ClI
**SMILES:** Cc1ccc(I)cc1Cl
**Mol. weight [g/mol]:** 252.48
**CAS:** 83846-48-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 147.40 | kJ/mol | Joback Method |
| hf | 86.91 | kJ/mol | Joback Method |
| hfus | 15.75 | kJ/mol | Joback Method |
| hvap | 48.53 | kJ/mol | Joback Method |
| log10ws | -3.78 | | Crippen Method |
| logp | 3.253 | | Crippen Method |
| mcvol | 123.790 | ml/mol | McGowan Method |
| pc | 3682.02 | kPa | Joback Method |
| tb | 526.77 | K | Joback Method |
| tc | 786.63 | K | Joback Method |
| tf | 308.09 | K | Joback Method |
| vc | 0.457 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 203.36 | J/mol×K | 526.77 | Joback Method |
| cpg | 242.95 | J/mol×K | 743.32 | Joback Method |
| cpg | 236.27 | J/mol×K | 700.01 | Joback Method |
| cpg | 229.02 | J/mol×K | 656.70 | Joback Method |
| cpg | 221.15 | J/mol×K | 613.39 | Joback Method |
| cpg | 212.62 | J/mol×K | 570.08 | Joback Method |
| cpg | 249.10 | J/mol×K | 786.63 | Joback Method |
| dvisc | 0.0003071 | Pa×s | 526.77 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003756 | Pa×s | 490.32 | Joback Method |
| dvisc | 0.0004745 | Pa×s | 453.88 | Joback Method |
| dvisc | 0.0006244 | Pa×s | 417.43 | Joback Method |
| dvisc | 0.0008661 | Pa×s | 380.98 | Joback Method |
| dvisc | 0.0012872 | Pa×s | 344.54 | Joback Method |
| dvisc | 0.0021012 | Pa×s | 308.09 | 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=C83846484&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 |
| **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 |