# Benzene, 4-iodo-1,2-dimethyl-

**Other names:** 1,2-Dimethyl-4-iodobenzene
**Inchi:** InChI=1S/C8H9I/c1-6-3-4-8(9)5-7(6)2/h3-5H,1-2H3
**InchiKey:** CSFRCLYFVINMBZ-UHFFFAOYSA-N
**Formula:** C8H9I
**SMILES:** Cc1ccc(I)cc1C
**Mol. weight [g/mol]:** 232.06
**CAS:** 31599-61-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 167.75 | kJ/mol | Joback Method |
| hf | 82.01 | kJ/mol | Joback Method |
| hfus | 14.14 | kJ/mol | Joback Method |
| hvap | 46.38 | kJ/mol | Joback Method |
| log10ws | -3.57 | | Crippen Method |
| logp | 2.908 | | Crippen Method |
| mcvol | 125.640 | ml/mol | McGowan Method |
| pc | 3431.89 | kPa | Joback Method |
| tb | 504.70 | K | NIST Webbook |
| tc | 761.77 | K | Joback Method |
| tf | 289.44 | K | Joback Method |
| vc | 0.464 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 222.94 | J/mol×K | 512.22 | Joback Method |
| cpg | 272.63 | J/mol×K | 720.18 | Joback Method |
| cpg | 264.08 | J/mol×K | 678.59 | Joback Method |
| cpg | 254.87 | J/mol×K | 637.00 | Joback Method |
| cpg | 244.98 | J/mol×K | 595.40 | Joback Method |
| cpg | 234.35 | J/mol×K | 553.81 | Joback Method |
| cpg | 280.59 | J/mol×K | 761.77 | Joback Method |
| dvisc | 0.0002884 | Pa×s | 512.22 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003543 | Pa×s | 475.09 | Joback Method |
| dvisc | 0.0004508 | Pa×s | 437.96 | Joback Method |
| dvisc | 0.0005998 | Pa×s | 400.83 | Joback Method |
| dvisc | 0.0008460 | Pa×s | 363.70 | Joback Method |
| dvisc | 0.0012902 | Pa×s | 326.57 | Joback Method |
| dvisc | 0.0021926 | Pa×s | 289.44 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 384.20 | K | 1.50 | NIST Webbook |

# Sources

**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=C31599618&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
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume