# 1-Methoxy-1,3-cyclohexadiene

**Other names:** 1,3-Cyclohexadiene, 1-methoxy-
1-methoxycyclohexa-1,3-diene
**Inchi:** InChI=1S/C7H10O/c1-8-7-5-3-2-4-6-7/h2-3,5H,4,6H2,1H3
**InchiKey:** LNRUJSUKKBJFOM-UHFFFAOYSA-N
**Formula:** C7H10O
**SMILES:** COC1=CC=CCC1
**Mol. weight [g/mol]:** 110.15
**CAS:** 2161-90-2

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -14.49 | kJ/mol | Joback Method |
| hf | -141.28 | kJ/mol | Joback Method |
| hfus | 7.89 | kJ/mol | Joback Method |
| hvap | 35.57 | kJ/mol | Joback Method |
| log10ws | -1.94 | | Crippen Method |
| logp | 1.867 | | Crippen Method |
| mcvol | 95.900 | ml/mol | McGowan Method |
| pc | 3848.31 | kPa | Joback Method |
| rinpol | 904.00 | | NIST Webbook |
| ripol | 1250.00 | | NIST Webbook |
| ripol | 1253.00 | | NIST Webbook |
| ripol | 1250.00 | | NIST Webbook |
| ripol | 1253.00 | | NIST Webbook |
| tb | 409.50 | K | Joback Method |
| tc | 618.03 | K | Joback Method |
| tf | 216.54 | K | Joback Method |
| vc | 0.351 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 173.00 | J/mol×K | 409.50 | Joback Method |
| cpg | 185.38 | J/mol×K | 444.25 | Joback Method |

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|---|---|---|---|---|
| cpg | 197.19 | J/mol×K | 479.01 | Joback Method |
| cpg | 208.43 | J/mol×K | 513.76 | Joback Method |
| cpg | 219.11 | J/mol×K | 548.52 | Joback Method |
| cpg | 229.25 | J/mol×K | 583.27 | Joback Method |
| cpg | 238.85 | J/mol×K | 618.03 | Joback Method |
| dvisc | 0.0031599 | Pa×s | 216.54 | Joback Method |
| dvisc | 0.0015242 | Pa×s | 248.70 | Joback Method |
| dvisc | 0.0008688 | Pa×s | 280.86 | Joback Method |
| dvisc | 0.0005559 | Pa×s | 313.02 | Joback Method |
| dvisc | 0.0003865 | Pa×s | 345.18 | Joback Method |
| dvisc | 0.0002859 | Pa×s | 377.34 | Joback Method |
| dvisc | 0.0002218 | Pa×s | 409.50 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 313.20 | K | 2.00 | 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=C2161902&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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |