# Cyclohexene, 3-(1-methylethyl)-

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|---|---|
| **Other names:** | 3-isopropylcyclohexene |
| | 3-Isopropylcyclohexene-1 |
| **Inchi:** | InChI=1S/C9H16/c1-8(2)9-6-4-3-5-7-9/h4,6,8-9H,3,5,7H2,1-2H3 |
| **InchiKey:** | HKZXDFQIKRFLMW-UHFFFAOYSA-N |
| **Formula:** | C9H16 |
| **SMILES:** | CC(C)C1C=CCCC1 |
| **Mol. weight [g/mol]:** | 124.22 |
| **CAS:** | 3983-08-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 76.87 | kJ/mol | Joback Method |
| hf | -122.27 | kJ/mol | Joback Method |
| hfus | 8.60 | kJ/mol | Joback Method |
| hvap | 35.96 | kJ/mol | Joback Method |
| log10ws | -2.85 | | Crippen Method |
| logp | 2.999 | | Crippen Method |
| mcvol | 122.510 | ml/mol | McGowan Method |
| pc | 2976.29 | kPa | Joback Method |
| rinpol | 948.00 | | NIST Webbook |
| rinpol | 921.00 | | NIST Webbook |
| rinpol | 926.10 | | NIST Webbook |
| rinpol | 924.00 | | NIST Webbook |
| rinpol | 926.50 | | NIST Webbook |
| rinpol | 956.00 | | NIST Webbook |
| rinpol | 915.90 | | NIST Webbook |
| rinpol | 921.00 | | NIST Webbook |
| ripol | 1093.00 | | NIST Webbook |
| ripol | 1070.00 | | NIST Webbook |
| ripol | 1081.00 | | NIST Webbook |
| ripol | 1062.80 | | NIST Webbook |
| ripol | 1043.80 | | NIST Webbook |
| ripol | 1053.90 | | NIST Webbook |
| ripol | 1081.00 | | NIST Webbook |
| ripol | 1049.00 | | NIST Webbook |
| tb | 423.59 | K | Joback Method |
| tc | 629.46 | K | Joback Method |

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|---|---|---|---|
| tf | 184.33 | K | Joback Method |
| vc | 0.453 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 241.39 | J/mol×K | 423.59 | Joback Method |
| cpg | 259.26 | J/mol×K | 457.90 | Joback Method |
| cpg | 276.23 | J/mol×K | 492.21 | Joback Method |
| cpg | 292.30 | J/mol×K | 526.53 | Joback Method |
| cpg | 307.52 | J/mol×K | 560.84 | Joback Method |
| cpg | 321.90 | J/mol×K | 595.15 | Joback Method |
| cpg | 335.48 | J/mol×K | 629.46 | Joback Method |
| dvisc | 0.0107110 | Pa×s | 184.33 | Joback Method |
| dvisc | 0.0032873 | Pa×s | 224.21 | Joback Method |
| dvisc | 0.0014413 | Pa×s | 264.08 | Joback Method |
| dvisc | 0.0007846 | Pa×s | 303.96 | Joback Method |
| dvisc | 0.0004918 | Pa×s | 343.84 | Joback Method |
| dvisc | 0.0003397 | Pa×s | 383.71 | Joback Method |
| dvisc | 0.0002516 | Pa×s | 423.59 | Joback Method |

# 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=C3983082&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

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|---|---|
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |