# 3,5-Hexadien-2-ol, 2-methyl-

**Inchi:** InChI=1S/C7H12O/c1-4-5-6-7(2,3)8/h4-6,8H,1H2,2-3H3/b6-5+
**InchiKey:** ZWRDKAOHFSUWQC-AATRIKPKSA-N
**Formula:** C7H12O
**SMILES:** C=CC=CC(C)(C)O
**Mol. weight [g/mol]:** 112.17
**CAS:** 926-38-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 42.14 | kJ/mol | Joback Method |
| hf | -106.14 | kJ/mol | Joback Method |
| hfus | 9.48 | kJ/mol | Joback Method |
| hvap | 45.85 | kJ/mol | Joback Method |
| log10ws | -1.84 | | Crippen Method |
| logp | 1.499 | | Crippen Method |
| mcvol | 106.760 | ml/mol | McGowan Method |
| pc | 3522.09 | kPa | Joback Method |
| tb | 449.35 | K | Joback Method |
| tc | 630.97 | K | Joback Method |
| tf | 225.05 | K | Joback Method |
| vc | 0.397 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 217.90 | J/mol×K | 449.35 | Joback Method |
| cpg | 228.54 | J/mol×K | 479.62 | Joback Method |
| cpg | 238.54 | J/mol×K | 509.89 | Joback Method |
| cpg | 247.93 | J/mol×K | 540.16 | Joback Method |
| cpg | 256.75 | J/mol×K | 570.43 | Joback Method |
| cpg | 265.03 | J/mol×K | 600.70 | Joback Method |
| cpg | 272.82 | J/mol×K | 630.97 | Joback Method |
| dvisc | 0.0990503 | Pa×s | 225.05 | Joback Method |
| dvisc | 0.0164039 | Pa×s | 262.43 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0042538 | Pa×s | 299.82 | Joback Method |
| dvisc | 0.0014879 | Pa×s | 337.20 | Joback Method |
| dvisc | 0.0006419 | Pa×s | 374.58 | Joback Method |
| dvisc | 0.0003225 | Pa×s | 411.97 | Joback Method |
| dvisc | 0.0001817 | Pa×s | 449.35 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C926385&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 |