# 1,4-Heptadien-3-ol, 3-methyl-6-(4-methylphenyl)

**Inchi:** InChI=1S/C15H20O/c1-5-15(4,16)11-10-13(3)14-8-6-12(2)7-9-14/h5-11,13,16H,1H2,2-4H

**InchiKey:** PWPWYHFOHOPRRH-ZHACJKMWSA-N

**Formula:** C15H20O

**SMILES:** C=CC(C)(O)C=CC(C)c1ccc(C)cc1

**Mol. weight [g/mol]:** 216.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 209.84 | kJ/mol | Joback Method |
| hf | -51.48 | kJ/mol | Joback Method |
| hfus | 20.33 | kJ/mol | Joback Method |
| hvap | 66.20 | kJ/mol | Joback Method |
| log10ws | -4.31 | | Crippen Method |
| logp | 3.592 | | Crippen Method |
| mcvol | 195.720 | ml/mol | McGowan Method |
| pc | 2206.22 | kPa | Joback Method |
| rinpol | 1510.00 | | NIST Webbook |
| rinpol | 1510.00 | | NIST Webbook |
| tb | 663.61 | K | Joback Method |
| tc | 869.55 | K | Joback Method |
| tf | 339.15 | K | Joback Method |
| vc | 0.731 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 519.14 | J/mol×K | 663.61 | Joback Method |
| cpg | 534.17 | J/mol×K | 697.93 | Joback Method |
| cpg | 548.23 | J/mol×K | 732.26 | Joback Method |
| cpg | 561.40 | J/mol×K | 766.58 | Joback Method |
| cpg | 573.75 | J/mol×K | 800.90 | Joback Method |
| cpg | 585.37 | J/mol×K | 835.22 | Joback Method |
| cpg | 596.32 | J/mol×K | 869.55 | Joback Method |
| dvisc | 0.0058689 | Pa×s | 339.15 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0013556 | Pa×s | 393.23 | Joback Method |
| dvisc | 0.0004463 | Pa×s | 447.30 | Joback Method |
| dvisc | 0.0001867 | Pa×s | 501.38 | Joback Method |
| dvisc | 0.0000925 | Pa×s | 555.46 | Joback Method |
| dvisc | 0.0000520 | Pa×s | 609.53 | Joback Method |
| dvisc | 0.0000321 | Pa×s | 663.61 | Joback Method |

# Sources

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|---|---|
| **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=R400109&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |