# 3-Hexene, 3-methoxy-2,5-dimethyl-, (E)-

**Inchi:** InChI=1S/C9H18O/c1-7(2)6-9(10-5)8(3)4/h6-8H,1-5H3/b9-6+
**InchiKey:** PYPPCCYSBRCXAF-RMKNXTFCSA-N
**Formula:** C9H18O
**SMILES:** COC(=CC(C)C)C(C)C
**Mol. weight [g/mol]:** 142.24
**CAS:** 66017-23-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -13.31 | kJ/mol | Joback Method |
| hf | -264.44 | kJ/mol | Joback Method |
| hfus | 12.10 | kJ/mol | Joback Method |
| hvap | 37.30 | kJ/mol | Joback Method |
| log10ws | -2.54 | | Crippen Method |
| logp | 2.829 | | Crippen Method |
| mcvol | 139.240 | ml/mol | McGowan Method |
| pc | 2436.25 | kPa | Joback Method |
| tb | 430.90 | K | Joback Method |
| tc | 613.21 | K | Joback Method |
| tf | 164.38 | K | Joback Method |
| vc | 0.526 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 283.59 | J/mol×K | 430.90 | Joback Method |
| cpg | 298.22 | J/mol×K | 461.28 | Joback Method |
| cpg | 312.26 | J/mol×K | 491.67 | Joback Method |
| cpg | 325.72 | J/mol×K | 522.05 | Joback Method |
| cpg | 338.60 | J/mol×K | 552.44 | Joback Method |
| cpg | 350.94 | J/mol×K | 582.82 | Joback Method |
| cpg | 362.73 | J/mol×K | 613.21 | Joback Method |

# Sources

| | |
|---|---|
| **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=C66017230&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |