# 1,6-Octadiene, 3-ethoxy-3,7-dimethyl-

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|---|---|
| **Other names:** | 3-Ethoxy-3,7-dimethyl-1,6-octadiene |
| | Ethyl linalool |
| | 3-ethoxy-3,7-dimethylocta-1,6-diene |
| | Ethoxylinalool |
| **Inchi:** | InChI=1S/C12H22O/c1-6-12(5,13-7-2)10-8-9-11(3)4/h6,9H,1,7-8,10H2,2-5H3 |
| **InchiKey:** | GSFBRCUXDDCNKV-UHFFFAOYSA-N |
| **Formula:** | C12H22O |
| **SMILES:** | C=CC(C)(CCC=C(C)C)OCC |
| **Mol. weight [g/mol]:** | 182.30 |
| **CAS:** | 72845-33-1 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 107.51 | kJ/mol | Joback Method |
| hf | -199.12 | kJ/mol | Joback Method |
| hfus | 18.22 | kJ/mol | Joback Method |
| hvap | 42.79 | kJ/mol | Joback Method |
| log10ws | -3.75 | | Crippen Method |
| logp | 3.714 | | Crippen Method |
| mcvol | 177.210 | ml/mol | McGowan Method |
| pc | 1942.37 | kPa | Joback Method |
| ripol | 1725.00 | | NIST Webbook |
| ripol | 1725.00 | | NIST Webbook |
| tb | 493.87 | K | Joback Method |
| tc | 677.89 | K | Joback Method |
| tf | 228.85 | K | Joback Method |
| vc | 0.676 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 403.04 | J/mol×K | 493.87 | Joback Method |
| cpg | 420.23 | J/mol×K | 524.54 | Joback Method |
| cpg | 436.55 | J/mol×K | 555.21 | Joback Method |

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|---|---|---|---|---|
| cpg | 452.04 | J/mol×K | 585.88 | Joback Method |
| cpg | 466.75 | J/mol×K | 616.55 | Joback Method |
| cpg | 480.70 | J/mol×K | 647.22 | Joback Method |
| cpg | 493.93 | J/mol×K | 677.89 | Joback Method |

# Sources

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|---|---|
| **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=C72845331&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |