

5,7-Octadien-2-ol, 2,6-dimethyl-

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|-----------------------------|--|
| Other names: | 2,6-Dimethyl-5,7-octadien-2-ol Ocimenol |
| Inchi: | InChI=1S/C10H18O/c1-5-9(2)7-6-8-10(3,4)11/h5,7,11H,1,6,8H2,2-4H3/b9-7+ |
| InchiKey: | IJKZRMIRAVXRK-VQHVLOKHSA-N |
| Formula: | C10H18O |
| SMILES: | <chem>C=CC(C)=CCCC(C)(C)O</chem> |
| Mol. weight [g/mol]: | 154.25 |
| CAS: | 5986-38-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | 58.85 | kJ/mol | Joback Method |
| hf | -177.85 | kJ/mol | Joback Method |
| hfus | 15.94 | kJ/mol | Joback Method |
| hvap | 52.61 | kJ/mol | Joback Method |
| log10ws | -3.09 | | Crippen Method |
| logp | 2.670 | | Crippen Method |
| mcvol | 149.030 | ml/mol | McGowan Method |
| pc | 2581.96 | kPa | Joback Method |
| rinpol | 1155.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1174.00 | | NIST Webbook |
| rinpol | 1155.00 | | NIST Webbook |
| rinpol | 1179.00 | | NIST Webbook |
| rinpol | 1139.00 | | NIST Webbook |
| rinpol | 1150.00 | | NIST Webbook |
| rinpol | 1179.00 | | NIST Webbook |
| rinpol | 1177.00 | | NIST Webbook |
| rinpol | 1153.00 | | NIST Webbook |
| rinpol | 1174.00 | | NIST Webbook |
| ripol | 1640.00 | | NIST Webbook |
| ripol | 1688.00 | | NIST Webbook |
| ripol | 1673.00 | | NIST Webbook |
| ripol | 1687.00 | | NIST Webbook |
| ripol | 1688.00 | | NIST Webbook |
| ripol | 1688.00 | | NIST Webbook |

| | | | |
|----|--------|----------------------|---------------|
| tb | 517.87 | K | Joback Method |
| tc | 697.57 | K | Joback Method |
| tf | 244.90 | K | Joback Method |
| vc | 0.566 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 347.03 | J/mol×K | 517.87 | Joback Method |
| cpg | 360.38 | J/mol×K | 547.82 | Joback Method |
| cpg | 372.99 | J/mol×K | 577.77 | Joback Method |
| cpg | 384.91 | J/mol×K | 607.72 | Joback Method |
| cpg | 396.18 | J/mol×K | 637.67 | Joback Method |
| cpg | 406.83 | J/mol×K | 667.62 | Joback Method |
| cpg | 416.91 | J/mol×K | 697.57 | Joback Method |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.42607e+01 |
| Coeff. B | -4.10698e+03 |
| Coeff. C | -7.48620e+01 |
| Temperature range (K), min. | 368.78 |
| Temperature range (K), max. | 533.78 |

Sources

| | |
|---|---|
| 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=C5986389&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| pvap: | Vapor 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 |

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