

# 2,7-Dimethyl-2,6-octadien-4-ol

|                      |                                                                 |
|----------------------|-----------------------------------------------------------------|
| Other names:         | 2,6-Octadien-4-ol, 2,7-dimethyl                                 |
| Inchi:               | InChI=1S/C10H18O/c1-8(2)5-6-10(11)7-9(3)4/h5,7,10-11H,6H2,1-4H3 |
| InchiKey:            | UJWFFQNWDJNWLH-UHFFFAOYSA-N                                     |
| Formula:             | C10H18O                                                         |
| SMILES:              | CC(C)=CCC(O)C=C(C)C                                             |
| Mol. weight [g/mol]: | 154.25                                                          |
| CAS:                 | 37665-99-9                                                      |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 37.40   | kJ/mol  | Joback Method  |
| hf            | -192.38 | kJ/mol  | Joback Method  |
| hfus          | 20.00   | kJ/mol  | Joback Method  |
| hvap          | 54.22   | kJ/mol  | Joback Method  |
| log10ws       | -3.09   |         | Crippen Method |
| logp          | 2.670   |         | Crippen Method |
| mcvol         | 149.030 | ml/mol  | McGowan Method |
| pc            | 2592.49 | kPa     | Joback Method  |
| tb            | 528.02  | K       | Joback Method  |
| tc            | 708.51  | K       | Joback Method  |
| tf            | 210.20  | K       | Joback Method  |
| vc            | 0.571   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 344.72 | J/mol×K | 528.02          | Joback Method |
| cpg           | 357.83 | J/mol×K | 558.10          | Joback Method |
| cpg           | 370.28 | J/mol×K | 588.18          | Joback Method |
| cpg           | 382.10 | J/mol×K | 618.27          | Joback Method |
| cpg           | 393.33 | J/mol×K | 648.35          | Joback Method |
| cpg           | 404.01 | J/mol×K | 678.43          | Joback Method |
| cpg           | 414.17 | J/mol×K | 708.51          | Joback Method |

# Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C37665999&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37665999&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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