

# Citronellyl 3-methyl-2-butenate

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C15H26O2/c1-12(2)7-6-8-14(5)9-10-17-15(16)11-13(3)4/h7,11,14H,6,8-10H2,1 |
| <b>InchiKey:</b>            | DCEUMOZSMAUPSP-AWEZLNQCLSA-N  |
| <b>Formula:</b>             | C15H26O2  |
| <b>SMILES:</b>              | CC(C)=CCCC(C)CCOC(=O)C=C(C)C  |
| <b>Mol. weight [g/mol]:</b> | 238.37  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -17.60  | kJ/mol               | Joback Method  |
| hf            | -388.15 | kJ/mol               | Joback Method  |
| hfus          | 31.65   | kJ/mol               | Joback Method  |
| hvap          | 57.83   | kJ/mol               | Joback Method  |
| log10ws       | -4.43   |                      | Crippen Method |
| logp          | 4.268   |                      | Crippen Method |
| mvol          | 221.050 | ml/mol               | McGowan Method |
| pc            | 1612.88 | kPa                  | Joback Method  |
| rinpol        | 1640.00 |                      | NIST Webbook   |
| rinpol        | 1640.00 |                      | NIST Webbook   |
| tb            | 626.53  | K                    | Joback Method  |
| tc            | 813.52  | K                    | Joback Method  |
| tf            | 277.89  | K                    | Joback Method  |
| vc            | 0.856   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 580.04 | J/mol×K | 626.53          | Joback Method |
| cpg           | 597.38 | J/mol×K | 657.69          | Joback Method |
| cpg           | 613.87 | J/mol×K | 688.86          | Joback Method |
| cpg           | 629.53 | J/mol×K | 720.02          | Joback Method |
| cpg           | 644.42 | J/mol×K | 751.19          | Joback Method |
| cpg           | 658.56 | J/mol×K | 782.35          | Joback Method |
| cpg           | 671.98 | J/mol×K | 813.52          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R589594&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R589594&amp;Units=SI</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>hvp:</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>rinp:</b>    | Non-polar retention indices                     |
| <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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