

# Linalol oxide (furanoid)

|                      |                                                                                                                                                                                                                                                             |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-(tetrahydro-5-methyl-5-vinyl-2-furyl)propan-2-ol<br>2-Furanmethanol, 5-ethenyltetrahydro-«alpha»,«alpha»,5-trimethyl-5-ethenyltetrahydro-«alpha»,«alpha»-5-trimethyl-2-furanmethanol<br>Epoxylinalool<br>Linalol oxide (furanoid)<br>furan linalool oxide |
| Inchi:               | InChI=1S/C10H18O2/c1-5-10(4)7-6-8(12-10)9(2,3)11/h5,8,11H,1,6-7H2,2-4H3                                                                                                                                                                                     |
| InchiKey:            | BRHDDEIRQPDPMG-UHFFFAOYSA-N                                                                                                                                                                                                                                 |
| Formula:             | C10H18O2                                                                                                                                                                                                                                                    |
| SMILES:              | C=CC1(C)CCC(C(C)(C)O)O1                                                                                                                                                                                                                                     |
| Mol. weight [g/mol]: | 170.25                                                                                                                                                                                                                                                      |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 13.74   | kJ/mol | Joback Method  |
| logp          | 1.881   |        | Crippen Method |
| mcvol         | 148.340 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 383.75 | J/mol×K | 551.63          | Joback Method |
| cpg           | 399.17 | J/mol×K | 585.07          | Joback Method |
| cpg           | 413.59 | J/mol×K | 618.51          | Joback Method |
| cpg           | 427.13 | J/mol×K | 651.95          | Joback Method |
| cpg           | 439.91 | J/mol×K | 685.39          | Joback Method |
| cpg           | 452.03 | J/mol×K | 718.83          | Joback Method |
| cpg           | 463.60 | J/mol×K | 752.27          | Joback Method |

## Sources

|                                  |                                                                                                                                               |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>                                     |
| <b>Crippen Method:</b>           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C60047178&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C60047178&amp;Units=SI</a> |
| <b>Joback Method:</b>            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |

## Legend

|               |                                           |
|---------------|-------------------------------------------|
| <b>cpg:</b>   | Ideal gas heat capacity                   |
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions |
| <b>logp:</b>  | Octanol/Water partition coefficient       |
| <b>mcvol:</b> | McGowan's characteristic volume           |

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