

# cis-furan Linalool oxide

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C10H18O2/c1-5-10(4)7-6-8(12-10)9(2,3)11/h5,8,11H,1,6-7H2,2-4H3/t8-,10-/m0 |
| <b>InchiKey:</b>            | BRHDDEIRQPDPMG-WPRPVWTQSA-N  |
| <b>Formula:</b>             | C10H18O2   |
| <b>SMILES:</b>              | C=CC1(C)CCC(C(C)(C)O)O1  |
| <b>Mol. weight [g/mol]:</b> | 170.25   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -75.59  | kJ/mol               | Joback Method  |
| hf            | -361.90 | kJ/mol               | Joback Method  |
| hfus          | 13.74   | kJ/mol               | Joback Method  |
| hvap          | 55.87   | kJ/mol               | Joback Method  |
| log10ws       | -2.44   |                      | Crippen Method |
| logp          | 1.881   |                      | Crippen Method |
| mvol          | 148.340 | ml/mol               | McGowan Method |
| pc            | 2947.28 | kPa                  | Joback Method  |
| ripol         | 1467.00 |                      | NIST Webbook   |
| ripol         | 1464.00 |                      | NIST Webbook   |
| tb            | 551.63  | K                    | Joback Method  |
| tc            | 752.27  | K                    | Joback Method  |
| tf            | 321.07  | K                    | Joback Method  |
| vc            | 0.543   | m <sup>3</sup> /kmol | Joback 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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R611042&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R611042&amp;Units=SI</a> |
| <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.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>                     |

# 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>ripl:</b>    | 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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