

# 3-Octanol, 3,7-dimethyl-

|                      |                                                                                                                                                                                                                           |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Linalool tetrahydride<br>Tetrahydrolinalool<br>2,6-Dimethyl-6-octanol<br>3,7-Dimethyloctan-3-ol<br>3,7-Dimethyl-3-octanol<br>3,7-Dimethyloctanol-3<br>NSC 128151<br>Dihydrolinalool<br>3-Octanol, 3,7-dimethyl-, (.+/-.)- |
| Inchi:               | InChI=1S/C10H22O/c1-5-10(4,11)8-6-7-9(2)3/h9,11H,5-8H2,1-4H3                                                                                                                                                              |
| InchiKey:            | DLHQZZUEERVIGQ-UHFFFAOYSA-N                                                                                                                                                                                               |
| Formula:             | C10H22O                                                                                                                                                                                                                   |
| SMILES:              | CCC(C)(O)CCCC(C)C                                                                                                                                                                                                         |
| Mol. weight [g/mol]: | 158.28                                                                                                                                                                                                                    |
| CAS:                 | 57706-88-4                                                                                                                                                                                                                |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | -103.10       | kJ/mol  | Joback Method  |
| hf            | -415.99       | kJ/mol  | Joback Method  |
| hfus          | 14.81         | kJ/mol  | Joback Method  |
| hvap          | 52.85         | kJ/mol  | Joback Method  |
| log10ws       | -3.14         |         | Crippen Method |
| logp          | 2.974         |         | Crippen Method |
| mcvol         | 157.630       | ml/mol  | McGowan Method |
| pc            | 2358.78       | kPa     | Joback Method  |
| tb            | 469.40 ± 4.00 | K       | NIST Webbook   |
| tc            | 686.53        | K       | Joback Method  |
| tf            | 250.70        | K       | Joback Method  |
| vc            | 0.598         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 383.78    | J/mol×K | 516.71 | Joback Method |
| cpg   | 449.39    | J/mol×K | 658.22 | Joback Method |
| cpg   | 437.50    | J/mol×K | 629.92 | Joback Method |
| cpg   | 425.02    | J/mol×K | 601.62 | Joback Method |
| cpg   | 411.92    | J/mol×K | 573.32 | Joback Method |
| cpg   | 398.19    | J/mol×K | 545.01 | Joback Method |
| cpg   | 460.72    | J/mol×K | 686.53 | Joback Method |
| dvisc | 0.0001136 | Pa×s    | 516.71 | Joback Method |
| dvisc | 0.0002050 | Pa×s    | 472.38 | Joback Method |
| dvisc | 0.0004181 | Pa×s    | 428.04 | Joback Method |
| dvisc | 0.0010052 | Pa×s    | 383.71 | Joback Method |
| dvisc | 0.0030395 | Pa×s    | 339.37 | Joback Method |
| dvisc | 0.0128169 | Pa×s    | 295.03 | Joback Method |
| dvisc | 0.0899105 | Pa×s    | 250.70 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 345.20 | K    | 0.80           | NIST Webbook |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57706884&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57706884&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                         |
| McGowan Method: | <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>dvisc:</b> | Dynamic viscosity                            |
| <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>h<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log10 of Water solubility in mol/l              |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</b>              | McGowan's characteristic volume                 |
| <b>p<sub>c</sub>:</b>                 | Critical Pressure                               |
| <b>t<sub>b</sub>:</b>                 | Normal Boiling Point Temperature                |
| <b>t<sub>brp</sub>:</b>               | Boiling point at reduced pressure               |
| <b>t<sub>c</sub>:</b>                 | Critical Temperature                            |
| <b>t<sub>f</sub>:</b>                 | Normal melting (fusion) point                   |
| <b>v<sub>c</sub>:</b>                 | Critical Volume                                 |

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