

# 2,7-Octadiene-1,6-diol, 2,6-dimethyl-, (Z)-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | (2Z)-2,6-Dimethyl-2,7-octadiene-1,6-diol<br>2,6-Dimethyl-2(Z),7-octadiene-1,6-diol<br>cis-8-Hydroxylinalool<br>(Z)-2,6-Dimethyl-2,7-octadiene-1,6-diol<br>(Z)-2,6-Dimethyl-2,7-octadien-1,6-diol<br>(Z)-2,6-Dimethylocta-2,7-diene-1,6-diol<br>(Z)-8-Hydroxylinalol<br>cis-3,7-Dimethyl-1,6-octadiene-3,8-diol<br>(Z)-2,6-dimethyl-octa-2,7-dien-1,6-diol<br>(Z)-8-hydroxylinalool<br>(Z)-2,6-dimethyl-2,7- octadiene-1,6-diol<br>cis-8-hydroxylinalool (cis-3,7-dimethyl-1,6-octadiene-3,8-diol) |
| <b>Inchi:</b>               | InChI=1S/C10H18O2/c1-4-10(3,12)7-5-6-9(2)8-11/h4,6,11-12H,1,5,7-8H2,2-3H3/b9-6-   |
| <b>InchiKey:</b>            | NSMIMJYEKVSYMT-TWGQIWQCSA-N   |
| <b>Formula:</b>             | C10H18O2  |
| <b>SMILES:</b>              | C=CC(C)(O)CCC=C(C)CO  |
| <b>Mol. weight [g/mol]:</b> | 170.25  |
| <b>CAS:</b>                 | 103619-06-3   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -77.97  | kJ/mol | Joback Method  |
| hf            | -330.08 | kJ/mol | Joback Method  |
| hfus          | 20.03   | kJ/mol | Joback Method  |
| hvap          | 69.28   | kJ/mol | Joback Method  |
| log10ws       | -2.35   |        | Crippen Method |
| logp          | 1.642   |        | Crippen Method |
| mcvol         | 154.900 | ml/mol | McGowan Method |
| pc            | 2841.41 | kPa    | Joback Method  |
| rinpol        | 1361.00 |        | NIST Webbook   |
| rinpol        | 1358.00 |        | NIST Webbook   |
| rinpol        | 1362.00 |        | NIST Webbook   |
| rinpol        | 1357.00 |        | NIST Webbook   |
| rinpol        | 1360.00 |        | NIST Webbook   |
| rinpol        | 1357.00 |        | NIST Webbook   |
| rinpol        | 1362.00 |        | NIST Webbook   |
| rinpol        | 1361.00 |        | NIST Webbook   |

|       |         |                      |               |
|-------|---------|----------------------|---------------|
| ripol | 1357.00 |                      | NIST Webbook  |
| ripol | 1358.00 |                      | NIST Webbook  |
| ripol | 1370.00 |                      | NIST Webbook  |
| ripol | 2326.00 |                      | NIST Webbook  |
| ripol | 2327.00 |                      | NIST Webbook  |
| ripol | 2310.00 |                      | NIST Webbook  |
| ripol | 2343.00 |                      | NIST Webbook  |
| ripol | 2316.00 |                      | NIST Webbook  |
| ripol | 2327.00 |                      | NIST Webbook  |
| ripol | 2325.00 |                      | NIST Webbook  |
| ripol | 2311.00 |                      | NIST Webbook  |
| ripol | 2327.00 |                      | NIST Webbook  |
| ripol | 2310.00 |                      | NIST Webbook  |
| ripol | 2317.00 |                      | NIST Webbook  |
| ripol | 2327.00 |                      | NIST Webbook  |
| ripol | 2312.00 |                      | NIST Webbook  |
| ripol | 2344.00 |                      | NIST Webbook  |
| ripol | 2310.00 |                      | NIST Webbook  |
| tb    | 610.05  | K                    | Joback Method |
| tc    | 782.91  | K                    | Joback Method |
| tf    | 305.72  | K                    | Joback Method |
| vc    | 0.585   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 402.74 | J/mol×K | 610.05          | Joback Method |
| cpg           | 413.76 | J/mol×K | 638.86          | Joback Method |
| cpg           | 424.19 | J/mol×K | 667.67          | Joback Method |
| cpg           | 434.07 | J/mol×K | 696.48          | Joback Method |
| cpg           | 443.45 | J/mol×K | 725.29          | Joback Method |
| cpg           | 452.35 | J/mol×K | 754.10          | Joback Method |
| cpg           | 460.83 | J/mol×K | 782.91          | Joback Method |

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

|                        |   |
|------------------------|---|
| <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=C103619063&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C103619063&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>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>ripol:</b>   | Non-polar retention indices                     |
| <b>ripol:</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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