

# 4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | (. +/-)-Lavandulol<br>2-Isopropenyl-5-methylhex-4-en-1-ol           |
| <b>Inchi:</b>               | InChI=1S/C10H18O/c1-8(2)5-6-10(7-11)9(3)4/h5,10-11H,3,6-7H2,1-2,4H3 |
| <b>InchiKey:</b>            | CZVXBFUKBZRMKR-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C10H18O   |
| <b>SMILES:</b>              | C=C(C)C(CO)CC=C(C)C   |
| <b>Mol. weight [g/mol]:</b> | 154.25  |
| <b>CAS:</b>                 | 58461-27-1  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 45.02   | kJ/mol               | Joback Method  |
| hf            | -184.17 | kJ/mol               | Joback Method  |
| hfus          | 18.52   | kJ/mol               | Joback Method  |
| hvap          | 53.59   | kJ/mol               | Joback Method  |
| log10ws       | -2.74   |                      | Crippen Method |
| logp          | 2.527   |                      | Crippen Method |
| mvol          | 149.030 | ml/mol               | McGowan Method |
| pc            | 2566.29 | kPa                  | Joback Method  |
| rinpol        | 1170.30 |                      | NIST Webbook   |
| tb            | 520.54  | K                    | Joback Method  |
| tc            | 696.89  | K                    | Joback Method  |
| tf            | 213.52  | K                    | Joback Method  |
| vc            | 0.572   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 343.99 | J/molxK | 520.54          | Joback Method |
| cpg           | 356.95 | J/molxK | 549.93          | Joback Method |
| cpg           | 369.29 | J/molxK | 579.32          | Joback Method |
| cpg           | 381.04 | J/molxK | 608.71          | Joback Method |
| cpg           | 392.23 | J/molxK | 638.10          | Joback Method |
| cpg           | 402.88 | J/molxK | 667.49          | 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.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>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C58461271&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58461271&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>rinpol:</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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