

# «beta»-Isocyclolavandulol

|                      |                                                                            |
|----------------------|----------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C10H18O/c1-8-6-10(2,3)5-4-9(8)7-11/h4,8,11H,5-7H2,1-3H3/t8-/m0/s1 |
| InchiKey:            | OEULXMGLLLUSOX-QMMMGPBSA-N                                                 |
| Formula:             | C10H18O                                                                    |
| SMILES:              | CC1CC(C)(C)CC=C1CO                                                         |
| Mol. weight [g/mol]: | 154.25                                                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -71.92  | kJ/mol  | Joback Method  |
| hf            | -306.43 | kJ/mol  | Joback Method  |
| hfus          | 13.18   | kJ/mol  | Joback Method  |
| hvap          | 54.46   | kJ/mol  | Joback Method  |
| log10ws       | -2.54   |         | Crippen Method |
| logp          | 2.361   |         | Crippen Method |
| mcvol         | 142.470 | ml/mol  | McGowan Method |
| pc            | 2928.17 | kPa     | Joback Method  |
| rinpol        | 1163.00 |         | NIST Webbook   |
| ripol         | 1759.00 |         | NIST Webbook   |
| tb            | 539.64  | K       | Joback Method  |
| tc            | 735.52  | K       | Joback Method  |
| tf            | 303.60  | K       | Joback Method  |
| vc            | 0.530   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 350.85 | J/mol×K | 539.64          | Joback Method |
| cpg           | 366.02 | J/mol×K | 572.29          | Joback Method |
| cpg           | 380.37 | J/mol×K | 604.93          | Joback Method |
| cpg           | 393.99 | J/mol×K | 637.58          | Joback Method |
| cpg           | 406.95 | J/mol×K | 670.22          | Joback Method |
| cpg           | 419.32 | J/mol×K | 702.87          | Joback Method |
| cpg           | 431.19 | J/mol×K | 735.52          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>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=R418858&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R418858&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>rinpola:</b> | Non-polar retention indices                     |
| <b>ripola:</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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