

# Muurola-4,10(14)-dien-8«beta»-ol

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H24O/c1-9(2)15-13-7-10(3)5-6-12(13)11(4)8-14(15)16/h7,9,12-16H,4-6,8H |
| InchiKey:            | UHPAOJOYWJZLCG-CVSAEHQPSA-N                                                       |
| Formula:             | C15H24O                                                                           |
| SMILES:              | C=C1CC(O)C(C(C)C)C2C=C(C)CCC12                                                    |
| Mol. weight [g/mol]: | 220.35                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 67.25   | kJ/mol  | Joback Method  |
| hf            | -299.61 | kJ/mol  | Joback Method  |
| hfus          | 24.86   | kJ/mol  | Joback Method  |
| hvap          | 66.28   | kJ/mol  | Joback Method  |
| log10ws       | -4.01   |         | Crippen Method |
| logp          | 3.552   |         | Crippen Method |
| mcvol         | 197.760 | ml/mol  | McGowan Method |
| pc            | 2021.76 | kPa     | Joback Method  |
| rinpol        | 1632.00 |         | NIST Webbook   |
| tb            | 658.86  | K       | Joback Method  |
| tc            | 858.82  | K       | Joback Method  |
| tf            | 344.91  | K       | Joback Method  |
| vc            | 0.739   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 577.43    | J/mol×K | 658.86          | Joback Method |
| cpg           | 596.53    | J/mol×K | 692.19          | Joback Method |
| cpg           | 614.55    | J/mol×K | 725.51          | Joback Method |
| cpg           | 631.52    | J/mol×K | 758.84          | Joback Method |
| cpg           | 647.47    | J/mol×K | 792.17          | Joback Method |
| cpg           | 662.43    | J/mol×K | 825.50          | Joback Method |
| cpg           | 676.45    | J/mol×K | 858.82          | Joback Method |
| dvisc         | 0.0046470 | Pa×s    | 344.91          | Joback Method |
| dvisc         | 0.0017837 | Pa×s    | 397.24          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008556 | Pa×s | 449.56 | Joback Method |
| dvisc | 0.0004784 | Pa×s | 501.88 | Joback Method |
| dvisc | 0.0002985 | Pa×s | 554.21 | Joback Method |
| dvisc | 0.0002020 | Pa×s | 606.54 | Joback Method |
| dvisc | 0.0001455 | Pa×s | 658.86 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R233206&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233206&amp;Units=SI</a> |
| <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>                     |

## 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>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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