

# «tau»-Cadinol

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7,8,8a-octahydro-1-naphthalenol-,<br>(1S-(1alpha,4alpha,4aalpha,8abeta))-<br>(1S,4S,4aR,8aR)-4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-ol<br>«alpha»-epi-Cadinol<br>10-epi-«alpha»-Cadinol<br>Cadinol, epi-«alpha»<br>Cadinol T<br>epi- «alpha»- «tau»-Cadinol<br>epi-«alpha»-Cadinol<br>T-Cadinol<br>1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-,<br>(1S-(1alpha,4alpha,4aalpha,8abeta))-<br>Cedrelanol<br>10-Epicadinol<br>1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-,<br>(1S,4S,4aR,8aR)-<br>1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-,<br>[1S-(1«alpha»,4«alpha»,4a«alpha»,8a«beta»)]-<br>10«beta»H-Cadin-4-en-10-ol<br>epi-Cadinol<br>10-epi-«alpha»-Cadinol (T-Cadinol)<br>epi-«alpha»-Cadinol («tau»-Cadinol)<br>epi-«alpha»-cadinol (T-cadinol)<br>T-Cadinol (10-epi-«alpha»-cadinol)<br>1-epi- «alpha»-Cadinol |
| Inchi:               | InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h9-10,12-14,16H,5-                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| InchiKey:            | LHYHMMRYTDARSZ-BARDWOONSA-N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| Formula:             | C15H26O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| SMILES:              | CC1=CC2C(C(C)C)CCC(C)(O)C2CC1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| Mol. weight [g/mol]: | 222.37                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| CAS:                 | 5937-11-1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | 8.68    | kJ/mol | Joback Method  |
| hf            | -368.61 | kJ/mol | Joback Method  |
| hfus          | 19.72   | kJ/mol | Joback Method  |
| hvap          | 64.97   | kJ/mol | Joback Method  |
| log10ws       | -4.15   |        | Crippen Method |
| logp          | 3.776   |        | Crippen Method |

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|--------|---------|--------|----------------|
| mcvol  | 202.060 | ml/mol | McGowan Method |
| pc     | 2069.88 | kPa    | Joback Method  |
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| tc    | 865.11  | K                    | Joback Method |
| tf    | 355.13  | K                    | Joback Method |
| vc    | 0.752   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
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| cpg           | 636.77 | J/mol×K | 728.33          | Joback Method |
| cpg           | 654.86 | J/mol×K | 762.52          | Joback Method |
| cpg           | 672.18 | J/mol×K | 796.72          | Joback Method |
| cpg           | 688.83 | J/mol×K | 830.91          | Joback Method |
| cpg           | 704.93 | J/mol×K | 865.11          | Joback Method |

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|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5937111&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5937111&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>                                       |

## 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>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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