

# Ethanol, 2-(3,3-dimethylcyclohexylidene)-, (z)-

|                      |                                                                                                                                                                                                                     |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (Z)-2-(3,3-Dimethylcyclohexylidene)ethanol<br>(2Z)-2-(3,3-Dimethylcyclohexylidene)ethanol<br>cis-3,3-dimethyl-«delta»1-«beta»-cyclohexanethanol<br>Grandlure II<br>Ethanol, 2-(3,3-dimethylcyclohexylidene)-, (2Z)- |
| Inchi:               | InChI=1S/C10H18O/c1-10(2)6-3-4-9(8-10)5-7-11/h5,11H,3-4,6-8H2,1-2H3/b9-5-                                                                                                                                           |
| InchiKey:            | SHYLMMBHTKLAJS-UITAMQMPSA-N                                                                                                                                                                                         |
| Formula:             | C10H18O                                                                                                                                                                                                             |
| SMILES:              | CC1(C)CCC/C(=C/CO)C1                                                                                                                                                                                                |
| Mol. weight [g/mol]: | 154.25                                                                                                                                                                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 11.60   | kJ/mol | Joback Method  |
| logp          | 2.505   |        | Crippen Method |
| mcvol         | 142.470 | ml/mol | McGowan Method |
| rinpol        | 1225.00 |        | NIST Webbook   |
| ripol         | 1865.00 |        | NIST Webbook   |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 349.74 | J/mol×K | 546.81          | Joback Method |
| cpg           | 364.83 | J/mol×K | 580.05          | Joback Method |
| cpg           | 379.05 | J/mol×K | 613.28          | Joback Method |
| cpg           | 392.50 | J/mol×K | 646.52          | Joback Method |
| cpg           | 405.27 | J/mol×K | 679.76          | Joback Method |
| cpg           | 417.46 | J/mol×K | 712.99          | Joback Method |
| cpg           | 429.16 | J/mol×K | 746.23          | Joback Method |

# Sources

|                                  |                                                                                                                                               |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b>           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>Cheméo Relay (1.0):</b>       |                                                                                                                                               |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                               |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C26532230&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C26532230&amp;Units=SI</a> |
| <b>Joback Method:</b>            | <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>hfus:</b>   | Enthalpy of fusion at standard conditions |
| <b>logp:</b>   | Octanol/Water partition coefficient       |
| <b>mcvol:</b>  | McGowan's characteristic volume           |
| <b>rinpol:</b> | Non-polar retention indices               |
| <b>ripol:</b>  | Polar retention indices                   |

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