

# endo-Fenchol

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | «alpha»-1,3,3-trimethyl bicyclo[2.2.1]heptan-2-ol                                  |
| <b>Inchi:</b>               | InChI=1S/C10H18O/c1-9(2)7-4-5-10(3,6-7)8(9)11/h7-8,11H,4-6H2,1-3H3/t7-,8-,10+/m0/s |
| <b>InchiKey:</b>            | IAIHUHQCLTYTSF-OYNCUSHFSA-N  |
| <b>Formula:</b>             | C10H18O  |
| <b>SMILES:</b>              | CC12CCC(C1)C(C)(C)C2O  |
| <b>Mol. weight [g/mol]:</b> | 154.25   |
| <b>CAS:</b>                 | 14575-74-7   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -20.50  | kJ/mol | Joback Method  |
| hf            | -272.72 | kJ/mol | Joback Method  |
| hfus          | 9.46    | kJ/mol | Joback Method  |
| hvap          | 51.61   | kJ/mol | Joback Method  |
| log10ws       | -2.45   |        | Crippen Method |
| logp          | 2.194   |        | Crippen Method |
| mcvol         | 135.910 | ml/mol | McGowan Method |
| pc            | 3166.83 | kPa    | Joback Method  |
| rinpol        | 1117.00 |        | NIST Webbook   |
| rinpol        | 1112.00 |        | NIST Webbook   |
| rinpol        | 1112.00 |        | NIST Webbook   |
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| rinpol        | 1117.00 |        | NIST Webbook   |
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| rinpol        | 1094.00 |        | NIST Webbook   |
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| rinpol        | 1113.00 |        | NIST Webbook   |
| rinpol        | 1103.00 |        | NIST Webbook   |

|        |         |                      |               |
|--------|---------|----------------------|---------------|
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| rinpol | 1134.00 |                      | NIST Webbook  |
| rinpol | 1116.00 |                      | NIST Webbook  |
| rinpol | 1111.00 |                      | NIST Webbook  |
| rinpol | 1114.00 |                      | NIST Webbook  |
| rinpol | 1120.00 |                      | NIST Webbook  |
| rinpol | 1112.00 |                      | NIST Webbook  |
| rinpol | 1111.00 |                      | NIST Webbook  |
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| rinpol | 1113.00 |                      | NIST Webbook  |
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| rinpol | 1088.00 |                      | NIST Webbook  |
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| rinpol | 1112.00 |                      | NIST Webbook  |
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| rinpol | 1118.00 |                      | NIST Webbook  |
| rinpol | 1111.00 |                      | NIST Webbook  |
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| rinpol | 1117.00 |                      | NIST Webbook  |
| rinpol | 1112.00 |                      | NIST Webbook  |
| rinpol | 1114.00 |                      | NIST Webbook  |
| rinpol | 1110.00 |                      | NIST Webbook  |
| rinpol | 1110.00 |                      | NIST Webbook  |
| rinpol | 1105.00 |                      | NIST Webbook  |
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| rinpol | 1119.00 |                      | NIST Webbook  |
| rinpol | 1094.00 |                      | NIST Webbook  |
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| ripol  | 1574.00 |                      | NIST Webbook  |
| ripol  | 1565.00 |                      | NIST Webbook  |
| ripol  | 1574.00 |                      | NIST Webbook  |
| ripol  | 1543.00 |                      | NIST Webbook  |
| tb     | 529.27  | K                    | Joback Method |
| tc     | 730.21  | K                    | Joback Method |
| tf     | 334.96  | K                    | Joback Method |
| vc     | 0.514   | m <sup>3</sup> /kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 354.30 | J/mol×K | 529.27          | Joback Method |
| cpg           | 370.25 | J/mol×K | 562.76          | Joback Method |
| cpg           | 385.05 | J/mol×K | 596.25          | Joback Method |
| cpg           | 398.92 | J/mol×K | 629.74          | Joback Method |
| cpg           | 412.02 | J/mol×K | 663.23          | Joback Method |
| cpg           | 424.55 | J/mol×K | 696.72          | Joback Method |
| cpg           | 436.70 | J/mol×K | 730.21          | 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=C14575747&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14575747&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>ripol:</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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