

# 1-cis-4-dimethyl-trans-2-ethylcyclopentane

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C9H18/c1-4-9-6-7(2)5-8(9)3/h7-9H,4-6H2,1-3H3/t7-,8+,9+/m0/s1 |
| <b>InchiKey:</b>            | VMCXXGFUCWAIIN-DJLDELDEBSA-N  |
| <b>Formula:</b>             | C9H18   |
| <b>SMILES:</b>              | CCC1CC(C)CC1C   |
| <b>Mol. weight [g/mol]:</b> | 126.24  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 46.03   | kJ/mol  | Joback Method  |
| hf            | -209.29 | kJ/mol  | Joback Method  |
| hfus          | 15.14   | kJ/mol  | Joback Method  |
| hvap          | 35.27   | kJ/mol  | Joback Method  |
| log10ws       | -2.76   |         | Crippen Method |
| logp          | 3.079   |         | Crippen Method |
| mcvol         | 126.810 | ml/mol  | McGowan Method |
| pc            | 2581.96 | kPa     | Joback Method  |
| rinpol        | 868.60  |         | NIST Webbook   |
| rinpol        | 873.80  |         | NIST Webbook   |
| rinpol        | 868.60  |         | NIST Webbook   |
| tb            | 411.26  | K       | Joback Method  |
| tc            | 601.43  | K       | Joback Method  |
| tf            | 193.61  | K       | Joback Method  |
| vc            | 0.478   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 255.59 | J/molxK | 411.26          | Joback Method |
| cpg           | 338.29 | J/molxK | 569.74          | Joback Method |
| cpg           | 323.20 | J/molxK | 538.04          | Joback Method |
| cpg           | 307.41 | J/molxK | 506.35          | Joback Method |
| cpg           | 290.88 | J/molxK | 474.65          | Joback Method |
| cpg           | 273.61 | J/molxK | 442.96          | Joback Method |
| cpg           | 352.67 | J/molxK | 601.43          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002834 | Paxs | 411.26 | Joback Method |
| dvisc | 0.0003244 | Paxs | 374.99 | Joback Method |
| dvisc | 0.0003821 | Paxs | 338.71 | Joback Method |
| dvisc | 0.0004681 | Paxs | 302.44 | Joback Method |
| dvisc | 0.0006061 | Paxs | 266.16 | Joback Method |
| dvisc | 0.0008515 | Paxs | 229.89 | Joback Method |
| dvisc | 0.0013588 | Paxs | 193.61 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=R164566&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R164566&amp;Units=SI</a> |
| <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>                         |

## 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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