

# 1-Oxaspiro[2.5]octan-4-one, 2,2,6-trimethyl-, trans-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | p-Menthan-3-one, 4,8-epoxy-, cis-cis-Pulegone Oxide<br>1-Oxaspiro[2.5]octan-4-one, 2,2,6-trimethyl-, (3R,6S)-rel-2,2,6-Trimethyl-1-oxaspiro[2.5]octan-4-one-, trans- |
| <b>Inchi:</b>               | InChI=1S/C10H16O2/c1-7-4-5-10(8(11)6-7)9(2,3)12-10/h7H,4-6H2,1-3H3/t7-,10+/m0/s1   |
| <b>InchiKey:</b>            | OFUGTKAUAMKFPM-OIBJUJFYSA-N  |
| <b>Formula:</b>             | C10H16O2   |
| <b>SMILES:</b>              | CC1CCC2(OC2(C)C)C(=O)C1  |
| <b>Mol. weight [g/mol]:</b> | 168.23   |
| <b>CAS:</b>                 | 13080-28-9   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -96.78  | kJ/mol  | Joback Method  |
| hf            | -376.01 | kJ/mol  | Joback Method  |
| hfus          | 9.69    | kJ/mol  | Joback Method  |
| hvap          | 44.17   | kJ/mol  | Joback Method  |
| log10ws       | -2.15   |         | Crippen Method |
| logp          | 1.923   |         | Crippen Method |
| mcvol         | 137.480 | ml/mol  | McGowan Method |
| pc            | 3138.51 | kPa     | Joback Method  |
| rinpol        | 1275.00 |         | NIST Webbook   |
| tb            | 540.80  | K       | Joback Method  |
| tc            | 780.01  | K       | Joback Method  |
| tf            | 369.65  | K       | Joback Method  |
| vc            | 0.516   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 356.06 | J/molxK | 540.80          | Joback Method |
| cpg           | 374.39 | J/molxK | 580.67          | Joback Method |
| cpg           | 391.40 | J/molxK | 620.54          | Joback Method |
| cpg           | 407.37 | J/molxK | 660.41          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 422.55 | J/mol×K | 700.27 | Joback Method |
| cpg | 437.20 | J/mol×K | 740.14 | Joback Method |
| cpg | 451.60 | J/mol×K | 780.01 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C13080289&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13080289&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>                                     |

## 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>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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