

# (-)-1R-8-Hydroxy-p-menth-4-en-3-one

|                      |                                                                                |
|----------------------|--------------------------------------------------------------------------------|
| Other names:         | 8-hydroxy-p-menth-4-en-3-one                                                   |
| Inchi:               | InChI=1S/C10H16O2/c1-7-4-5-8(9(11)6-7)10(2,3)12/h5,7,12H,4,6H2,1-3H3/t7-/m0/s1 |
| InchiKey:            | SNBPZAIQWQXUCR-ZETCQYMHSA-N                                                    |
| Formula:             | C10H16O2                                                                       |
| SMILES:              | CC1CC=C(C(C)(C)O)C(=O)C1                                                       |
| Mol. weight [g/mol]: | 168.23                                                                         |
| CAS:                 | 35736-66-4                                                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -178.47 | kJ/mol  | Joback Method  |
| hf            | -447.78 | kJ/mol  | Joback Method  |
| hfus          | 10.51   | kJ/mol  | Joback Method  |
| hvap          | 58.87   | kJ/mol  | Joback Method  |
| log10ws       | -2.17   |         | Crippen Method |
| logp          | 1.683   |         | Crippen Method |
| mcvol         | 144.040 | ml/mol  | McGowan Method |
| pc            | 3065.95 | kPa     | Joback Method  |
| rinpol        | 1264.00 |         | NIST Webbook   |
| tb            | 608.66  | K       | Joback Method  |
| tc            | 822.00  | K       | Joback Method  |
| tf            | 354.58  | K       | Joback Method  |
| vc            | 0.529   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 384.00 | J/mol×K | 608.66          | Joback Method |
| cpg           | 399.22 | J/mol×K | 644.22          | Joback Method |
| cpg           | 413.54 | J/mol×K | 679.77          | Joback Method |
| cpg           | 426.99 | J/mol×K | 715.33          | Joback Method |
| cpg           | 439.59 | J/mol×K | 750.88          | Joback Method |
| cpg           | 451.34 | J/mol×K | 786.44          | Joback Method |
| cpg           | 462.27 | J/mol×K | 822.00          | 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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C35736664&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35736664&amp;Units=SI</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>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>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>rinpola:</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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