

(-)-Myrtenol

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| Other names: | Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-, (1R)-(1R)-6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-methanol |
| Inchi: | InChI=1S/C10H16O/c1-10(2)8-4-3-7(6-11)9(10)5-8/h3,8-9,11H,4-6H2,1-2H3 |
| InchiKey: | RXBQNMWIKOSCS-UHFFFAOYSA-N |
| Formula: | C10H16O |
| SMILES: | CC1(C)C2CC=C(CO)C1C2 |
| Mol. weight [g/mol]: | 152.23 |
| CAS: | 19894-97-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 13.03 | kJ/mol | Joback Method |
| hf | -221.31 | kJ/mol | Joback Method |
| hfus | 15.52 | kJ/mol | Joback Method |
| hvap | 54.02 | kJ/mol | Joback Method |
| log10ws | -2.19 | | Crippen Method |
| logp | 1.971 | | Crippen Method |
| mcvol | 131.610 | ml/mol | McGowan Method |
| pc | 3199.16 | kPa | Joback Method |
| rinpol | 1212.80 | | NIST Webbook |
| rinpol | 1212.80 | | NIST Webbook |
| tb | 537.84 | K | Joback Method |
| tc | 734.16 | K | Joback Method |
| tf | 328.58 | K | Joback Method |
| vc | 0.503 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 335.67 | J/molxK | 537.84 | Joback Method |
| cpg | 349.94 | J/molxK | 570.56 | Joback Method |
| cpg | 363.29 | J/molxK | 603.28 | Joback Method |
| cpg | 375.84 | J/molxK | 636.00 | Joback Method |
| cpg | 387.71 | J/molxK | 668.72 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 399.00 | J/mol×K | 701.44 | Joback Method |
| cpg | 409.83 | J/mol×K | 734.16 | Joback Method |

Sources

| | |
|------------------------|---|
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C19894974&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|------------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpolar: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/70-199-4/Myrtenol.pdf>

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