

Salvial-4(14)-en-1-one

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| Other names: | Salvia-4(14)-en-1-one 4(14)-Salvialene-1-one Salvial-4(14)-en-1-on Salivial-4(14)-en-1-one Salvial-4(14)-en-1-one (mint ketone) |
| Inchi: | InChI=1S/C15H24O/c1-10(2)12-7-8-15(4)13(12)9-11(3)5-6-14(15)16/h10,12-13H,3,5-9H2 |
| InchiKey: | JBOONPKUPONSIB-UHFFFAOYSA-N |
| Formula: | C15H24O |
| SMILES: | <chem>C=C1CCC(=O)C2(C)CCC(C(C)C)C2C1</chem> |
| Mol. weight [g/mol]: | 220.35 |
| CAS: | 73809-82-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | 63.37 | kJ/mol | Joback Method |
| hf | -295.81 | kJ/mol | Joback Method |
| hfus | 12.08 | kJ/mol | Joback Method |
| hvap | 52.06 | kJ/mol | Joback Method |
| log10ws | -4.06 | | Crippen Method |
| logp | 3.984 | | Crippen Method |
| mcvol | 197.760 | ml/mol | McGowan Method |
| pc | 2021.76 | kPa | Joback Method |
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| ripol | 2016.00 | NIST Webbook |
| ripol | 2037.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C73809822&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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 |
| ripolar: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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