

(+)-(7S,10S)-Eudesma-4,11-dien-9-one

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|-----------------------------|--|
| Inchi: | InChI=1S/C15H22O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)14(16)9-12/h12H,1,5-9H2,2-4H |
| InchiKey: | VAIOFGRNCJWCNU-SWLSCSKDSA-N |
| Formula: | C15H22O |
| SMILES: | <chem>C=C(C)C1CC(=O)C2(C)CCCC(C)=C2C1</chem> |
| Mol. weight [g/mol]: | 218.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 110.43 | kJ/mol | Joback Method |
| hf | -203.95 | kJ/mol | Joback Method |
| hfus | 13.54 | kJ/mol | Joback Method |
| hvap | 53.62 | kJ/mol | Joback Method |
| log10ws | -4.39 | | Crippen Method |
| logp | 4.048 | | Crippen Method |
| mcvol | 193.460 | ml/mol | McGowan Method |
| pc | 2133.46 | kPa | Joback Method |
| rinsol | 1649.00 | | NIST Webbook |
| tb | 646.90 | K | Joback Method |
| tc | 885.57 | K | Joback Method |
| tf | 382.81 | K | Joback Method |
| vc | 0.731 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 538.47 | J/molxK | 646.90 | Joback Method |
| cpg | 560.03 | J/molxK | 686.68 | Joback Method |
| cpg | 580.39 | J/molxK | 726.46 | Joback Method |
| cpg | 599.70 | J/molxK | 766.24 | Joback Method |
| cpg | 618.11 | J/molxK | 806.02 | Joback Method |
| cpg | 635.78 | J/molxK | 845.79 | Joback Method |
| cpg | 652.86 | J/molxK | 885.57 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R561432&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

| | |
|-----------------|---|
| 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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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