# Methyl (E)-trans-«alpha»-bergamota-2,10-dien-12-oate

**Inchi:** InChI=1S/C16H24O2/c1-11-7-8-13-10-14(11)16(13,3)9-5-6-12(2)15(17)18-4/h6-7,13-14H

**InchiKey:** ZTBCGQOFWCYELA-SUCCEKNJSA-N

**Formula:** C16H24O2

**SMILES:** COC(=O)C(C)=CCCC1(C)C2CC=C(C)C1C2

**Mol. weight [g/mol]:** 248.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 38.12 | kJ/mol | Joback Method |
| hf | -330.29 | kJ/mol | Joback Method |
| hfus | 28.65 | kJ/mol | Joback Method |
| hvap | 59.90 | kJ/mol | Joback Method |
| log10ws | -4.15 | | Crippen Method |
| logp | 3.878 | | Crippen Method |
| mcvol | 213.420 | ml/mol | McGowan Method |
| pc | 1837.26 | kPa | Joback Method |
| rinpol | 1785.00 | | NIST Webbook |
| tb | 663.27 | K | Joback Method |
| tc | 872.43 | K | Joback Method |
| tf | 388.50 | K | Joback Method |
| vc | 0.826 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 604.93 | J/mol×K | 663.27 | Joback Method |
| cpg | 623.53 | J/mol×K | 698.13 | Joback Method |
| cpg | 641.22 | J/mol×K | 732.99 | Joback Method |
| cpg | 658.16 | J/mol×K | 767.85 | Joback Method |
| cpg | 674.47 | J/mol×K | 802.71 | Joback Method |
| cpg | 690.32 | J/mol×K | 837.57 | Joback Method |
| cpg | 705.85 | J/mol×K | 872.43 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R233711&Units=SI |

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