# trans-«alpha»-(Z)-Bergamotol

**Inchi:** InChI=1S/C15H24O/c1-11(10-16)5-4-8-15(3)13-7-6-12(2)14(15)9-13/h5-6,13-14,16H,4,7
**InchiKey:** JGINTSAQGRHGMG-KAIHXKKWSA-N
**Formula:** C15H24O
**SMILES:** CC(=CCCC1(C)C2CC=C(C)C1C2)CO
**Mol. weight [g/mol]:** 220.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 27.36 | kJ/mol | Joback Method |
| hvap | 94.11 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.10 | eV | Cheméo Relay (1.0) |
| logp | 3.698 | | Crippen Method |
| mcvol | 197.760 | ml/mol | McGowan Method |
| rinpol | 1606.00 | | NIST Webbook |
| tb | 577.53 | K | Cheméo Relay (1.0) |
| tf | 306.29 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 566.15 | J/mol×K | 656.28 | Joback Method |
| cpg | 582.77 | J/mol×K | 688.74 | Joback Method |
| cpg | 598.62 | J/mol×K | 721.20 | Joback Method |
| cpg | 613.83 | J/mol×K | 753.67 | Joback Method |
| cpg | 628.52 | J/mol×K | 786.13 | Joback Method |
| cpg | 642.83 | J/mol×K | 818.59 | Joback Method |
| cpg | 656.88 | J/mol×K | 851.05 | Joback Method |

## Sources

**Cheméo Relay (1.0, beta):**

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R613602&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |