# cis-«alpha»-Bergamotene

**Inchi:** InChI=1S/C15H24/c1-11(2)6-5-9-15(4)13-8-7-12(3)14(15)10-13/h6-7,13-14H,5,8-10H2,1-
**InchiKey:** YMBFCQPIMVLNIU-ZYOSVBKOSA-N
**Formula:** C15H24
**SMILES:** CC(C)=CCCC1(C)C2CC=C(C)C1C2
**Mol. weight [g/mol]:** 204.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 263.62 | kJ/mol | Joback Method |
| hf | -64.85 | kJ/mol | Joback Method |
| hfus | 23.27 | kJ/mol | Joback Method |
| hvap | 48.51 | kJ/mol | Joback Method |
| log10ws | -4.87 | | Crippen Method |
| logp | 4.725 | | Crippen Method |
| mcvol | 191.890 | ml/mol | McGowan Method |
| pc | 1918.62 | kPa | Joback Method |
| rinpol | 1412.00 | | NIST Webbook |
| rinpol | 1421.00 | | NIST Webbook |
| rinpol | 1419.00 | | NIST Webbook |
| rinpol | 1410.00 | | NIST Webbook |
| rinpol | 1412.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1413.00 | | NIST Webbook |
| rinpol | 1421.00 | | NIST Webbook |
| rinpol | 1413.00 | | NIST Webbook |
| rinpol | 1410.00 | | NIST Webbook |
| tb | 564.10 | K | Joback Method |
| tc | 771.48 | K | Joback Method |
| tf | 305.07 | K | Joback Method |
| vc | 0.746 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 496.98 | J/mol×K | 564.10 | Joback Method |
| cpg | 517.47 | J/mol×K | 598.66 | Joback Method |
| cpg | 536.69 | J/mol×K | 633.23 | Joback Method |
| cpg | 554.80 | J/mol×K | 667.79 | Joback Method |
| cpg | 571.95 | J/mol×K | 702.35 | Joback Method |
| cpg | 588.31 | J/mol×K | 736.92 | Joback Method |
| cpg | 604.03 | J/mol×K | 771.48 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R609722&Units=SI
**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

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

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