# cis-«alpha»-Bergamotene

**Other names:** «alpha»-cis-Bergamotene
(Z)-«alpha»-Bergamotene
cis-«alpha»-beramotene
«alpha»-Bergamotene cis
bergamotene (Z,«alpha»,cis)
«beta»-cis-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-UHFFFAOYSA-N
**Formula:** C15H24
**SMILES:** CC(C)=CCCC1(C)C2CC=C(C)C1C2
**Mol. weight [g/mol]:** 204.35
**CAS:** 18252-46-5

# 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 | 1409.00 | | NIST Webbook |
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| ripol | 1573.00 | | 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

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|---|---|
| **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=C18252465&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

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