# (-)-(5R,7S,10S)-cis-«beta»-Elemene

**Inchi:** InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5
**InchiKey:** OPFTUNCRGUEPRZ-ZNMIVQPWSA-N
**Formula:** C15H24
**SMILES:** C=CC1(C)CCC(C(=C)C)CC1C(=C)C
**Mol. weight [g/mol]:** 204.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 15.82 | kJ/mol | Joback Method |
| logp | 4.747 | | Crippen Method |
| mcvol | 198.450 | ml/mol | McGowan Method |
| rinpol | 1382.00 | | NIST Webbook |
| rinpol | 1382.00 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 488.78 | J/mol×K | 542.85 | Joback Method |
| cpg | 511.42 | J/mol×K | 578.06 | Joback Method |
| cpg | 532.71 | J/mol×K | 613.28 | Joback Method |
| cpg | 552.77 | J/mol×K | 648.49 | Joback Method |
| cpg | 571.73 | J/mol×K | 683.70 | Joback Method |
| cpg | 589.70 | J/mol×K | 718.92 | Joback Method |
| cpg | 606.82 | J/mol×K | 754.13 | Joback Method |

## Sources

**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R561645&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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |