# epi-«alpha»-Muurolol

**Inchi:** InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h9-10,12-14,16H,5-
**InchiKey:** LHYHMMRYTDARSZ-XSCHDIRWSA-N
**Formula:** C15H26O
**SMILES:** CC1=CC2C(C(C)C)CCC(C)(O)C2CC1
**Mol. weight [g/mol]:** 222.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -285.47 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 19.72 | kJ/mol | Joback Method |
| hvap | 82.40 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.36 | eV | Cheméo Relay (1.0) |
| logp | 3.776 | | Crippen Method |
| mcvol | 202.060 | ml/mol | McGowan Method |
| rinpol | 1642.00 | | NIST Webbook |
| rinpol | 1642.00 | | NIST Webbook |
| rinpol | 1655.00 | | NIST Webbook |
| rinpol | 1642.00 | | NIST Webbook |
| rinpol | 1644.00 | | NIST Webbook |
| rinpol | 1642.00 | | NIST Webbook |
| rinpol | 1648.00 | | NIST Webbook |
| rinpol | 1641.00 | | NIST Webbook |
| rinpol | 1640.00 | | NIST Webbook |
| rinpol | 1642.00 | | NIST Webbook |
| tb | 557.65 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 597.80 | J/mol×K | 659.94 | Joback Method |
| cpg | 617.79 | J/mol×K | 694.13 | Joback Method |
| cpg | 636.77 | J/mol×K | 728.33 | Joback Method |
| cpg | 654.86 | J/mol×K | 762.52 | Joback Method |
| cpg | 672.18 | J/mol×K | 796.72 | Joback Method |

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|---|---|---|---|---|
| cpg | 688.83 | J/mol×K | 830.91 | Joback Method |
| cpg | 704.93 | J/mol×K | 865.11 | Joback Method |

# Sources

| | |
|---|---|
| **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):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R600349&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **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 |