

# (-)-(1R,2S,6R,10S)-2.alpha.-Hydroxyamorpho-4,7(1

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | (-)-(1R,2S,6R,10S)-2«alpha»-Hydroxyamorpho-4,7(11)-diene                          |
| Inchi:               | InChI=1S/C15H24O/c1-9(2)12-6-5-11(4)15-13(12)7-10(3)8-14(15)16/h7,11,13-16H,5-6,8 |
| InchiKey:            | BEIGEIPJNFKPQA-CYUUQNCZSA-N                                                       |
| Formula:             | C15H24O                                                                           |
| SMILES:              | CC1=C[C@@H]2C(=C(C)C)CC[C@@H](C)[C@@H]2[C@H](O)C1                                 |
| Mol. weight [g/mol]: | 220.36                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 28.55   | kJ/mol | Joback Method  |
| logp          | 3.696   |        | Crippen Method |
| mcvol         | 197.760 | ml/mol | McGowan Method |
| rinpol        | 1684.00 |        | NIST Webbook   |
| rinpol        | 1684.00 |        | NIST Webbook   |
| rinpol        | 1684.00 |        | NIST Webbook   |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 578.39 | J/mol×K | 666.66          | Joback Method |
| cpg           | 597.44 | J/mol×K | 700.54          | Joback Method |
| cpg           | 615.40 | J/mol×K | 734.42          | Joback Method |
| cpg           | 632.32 | J/mol×K | 768.31          | Joback Method |
| cpg           | 648.22 | J/mol×K | 802.19          | Joback Method |
| cpg           | 663.16 | J/mol×K | 836.07          | Joback Method |
| cpg           | 677.18 | J/mol×K | 869.95          | Joback Method |

## Sources

|                 |                                                                                                                   |
|-----------------|-------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>         |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a> |

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R425415&Units=SI>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

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

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