

# .gamma.-Dehydro-ar-himachalene

|                      |                                                                                 |
|----------------------|---------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H20/c1-11-7-8-13-12(2)6-5-9-15(3,4)14(13)10-11/h6-8,10H,5,9H2,1-4H3 |
| InchiKey:            | KSQQTNWAKSYGCR-UHFFFAOYSA-N                                                     |
| Formula:             | C15H20                                                                          |
| SMILES:              | CC1=CCCC(C)(C)c2cc(C)ccc21                                                      |
| Mol. weight [g/mol]: | 200.33                                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | 12.95   | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 16.34   | kJ/mol | Joback Method      |
| logp          | 4.470   |        | Crippen Method     |
| mcvol         | 183.290 | ml/mol | McGowan Method     |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 460.71 | J/mol×K | 598.90          | Joback Method |
| cpg           | 480.03 | J/mol×K | 637.81          | Joback Method |
| cpg           | 498.17 | J/mol×K | 676.72          | Joback Method |
| cpg           | 515.30 | J/mol×K | 715.63          | Joback Method |
| cpg           | 531.57 | J/mol×K | 754.54          | Joback Method |
| cpg           | 547.15 | J/mol×K | 793.45          | Joback Method |
| cpg           | 562.19 | J/mol×K | 832.36          | Joback Method |

## Sources

|                     |                                                                                                                       |
|---------------------|-----------------------------------------------------------------------------------------------------------------------|
| Joback Method:      | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                 |
| McGowan Method:     | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a> |
| Crippen Method:     | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>             |
| Crippen Method:     | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C51766655&Units=SI>

## Legend

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

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