

# CHILOSCYPHONE

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H22O/c1-9(2)12-7-5-10(3)13-8-6-11(4)15(16)14(12)13/h5,9,12-14H,4,6-8H |
| InchiKey:            | VDMHNWBQSSGYNR-UHFFFAOYSA-N                                                       |
| Formula:             | C15H22O                                                                           |
| SMILES:              | C=C1CCC2C(C)=CCC(C(C)C)C2C1=O                                                     |
| Mol. weight [g/mol]: | 218.34                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 19.21   | kJ/mol | Joback Method  |
| logp          | 3.760   |        | Crippen Method |
| mccvol        | 193.460 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 543.23 | J/mol×K | 639.17          | Joback Method |
| cpg           | 565.16 | J/mol×K | 676.99          | Joback Method |
| cpg           | 585.76 | J/mol×K | 714.80          | Joback Method |
| cpg           | 605.04 | J/mol×K | 752.62          | Joback Method |
| cpg           | 623.01 | J/mol×K | 790.44          | Joback Method |
| cpg           | 639.71 | J/mol×K | 828.25          | Joback Method |
| cpg           | 655.13 | J/mol×K | 866.07          | Joback Method |

## Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23538456&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>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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           |

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