# HANPHYLLIN

**Inchi:** InChI=1S/C15H20O3/c1-9-4-6-12-11(3)15(17)18-14(12)8-10(2)13(16)7-5-9/h5,8,12-14,1
**InchiKey:** XQVSREKNQZKAKU-MUDDOMJDSA-N
**Formula:** C15H20O3
**SMILES:** C=C1C(=O)OC2/C=C(\C)C(O)C/C=C(\C)CCC12
**Mol. weight [g/mol]:** 248.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 29.33 | kJ/mol | Joback Method |
| logp | 2.522 | | Crippen Method |
| mcvol | 200.900 | ml/mol | McGowan Method |
| rinpol | 1966.00 | | NIST Webbook |
| rinpol | 1966.00 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 627.65 | J/mol×K | 775.69 | Joback Method |
| cpg | 644.79 | J/mol×K | 813.25 | Joback Method |
| cpg | 660.50 | J/mol×K | 850.82 | Joback Method |
| cpg | 674.78 | J/mol×K | 888.38 | Joback Method |
| cpg | 687.59 | J/mol×K | 925.94 | Joback Method |
| cpg | 698.93 | J/mol×K | 963.50 | Joback Method |
| cpg | 708.77 | J/mol×K | 1001.07 | Joback Method |

## Sources

**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

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C60268408&Units=SI

# 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 |