# Longiborneol acetate

**Inchi:** InChI=1S/C17H28O2/c1-11(18)19-14-13-12-7-10-17(14,5)16(12,4)9-6-8-15(13,2)3/h12-1
**InchiKey:** NVBYJWWRRWURRN-PKCNPWEKSA-N
**Formula:** C17H28O2
**SMILES:** CC(=O)OC1C2C3CCC1(C)C3(C)CCCC2(C)C
**Mol. weight [g/mol]:** 264.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 17.10 | kJ/mol | Joback Method |
| logp | 4.181 | | Crippen Method |
| mcvol | 225.250 | ml/mol | McGowan Method |
| rinpol | 1697.00 | | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 690.49 | J/mol×K | 680.12 | Joback Method |
| cpg | 713.37 | J/mol×K | 717.86 | Joback Method |
| cpg | 735.56 | J/mol×K | 755.59 | Joback Method |
| cpg | 757.45 | J/mol×K | 793.33 | Joback Method |
| cpg | 779.41 | J/mol×K | 831.06 | Joback Method |
| cpg | 801.82 | J/mol×K | 868.80 | Joback Method |
| cpg | 825.06 | J/mol×K | 906.53 | Joback Method |

## Sources

**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=R560706&Units=SI

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |