# Cacalohastine

**Inchi:** InChI=1S/C16H18O2/c1-9-6-5-7-12-13(9)11(3)14-10(2)8-18-16(14)15(12)17-4/h5,7-9H,6

**InchiKey:** WCJNJWNPAYBQPW-SECBINFHSA-N

**Formula:** C16H18O2

**SMILES:** COc1c2c(c(C)c3c(C)coc13)C(C)CC=C2

**Mol. weight [g/mol]:** 242.31

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -9.98 | | Crippen Method |
| logp | 4.579 | | Crippen Method |
| mcvol | 193.960 | ml/mol | McGowan Method |
| rinpol | 2055.00 | | NIST Webbook |
| rinpol | 2055.00 | | NIST Webbook |
| ripol | 2820.00 | | NIST Webbook |
| ripol | 2820.00 | | NIST Webbook |

# Sources

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

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R616092&Units=SI

# Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices

**ripol:** Polar retention indices