# Aposcopolamine

**Inchi:** InChI=1S/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-
**InchiKey:** STECJAGHUSJQJN-QBMZJCKTSA-N
**Formula:** C17H21NO4
**SMILES:** CN1C2CC(OC(=O)C(CO)c3ccccc3)CC1C1OC12
**Mol. weight [g/mol]:** 303.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.03 | | Crippen Method |
| logp | 0.918 | | Crippen Method |
| mcvol | 223.210 | ml/mol | McGowan Method |
| rinpol | 2130.00 | | NIST Webbook |
| rinpol | 2130.00 | | NIST Webbook |
| rinpol | 2130.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R411124&Units=SI
**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

## Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**rinpol:** Non-polar retention indices