Atropine acetate

Inchi: InChI=1S/C19H25NO4/c1-13(21)23-12-18(14-6-4-3-5-7-14)19(22)24-17-10-15-8-9-16(11
InchiKey: FFTQFHULPHYOIS-UHFFFAOYSA-N
Formula: C19H25NO4
SMILES: CC(=O)OCC(C(=O)OC1CC2CCC(C1)N2C)c1ccccc1
Mol. weight [g/mol]: 331.41
CAS: 535995-20-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.502		Crippen Method
mcvol	257.950	ml/mol	McGowan Method
rinpol	2355.50		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C535995201&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.