DL-Homatropine, methyl ether

Inchi: InChI=1S/C17H23NO3/c1-18-13-8-9-14(18)11-15(10-13)21-17(19)16(20-2)12-6-4-3-5-7-
InchiKey: UCEHPVVJPVFWAZ-UHFFFAOYSA-N
Formula: C17H23NO3
SMILES: COC(C(=O)OC1CC2CCC(C1)N2C)c1ccccc1
Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-1.42		Cheméo Relay (1.0)
logp	2.542		Crippen Method
mcvol	228.200	ml/mol	McGowan Method
rinpol	2143.10		NIST Webbook
rinpol	2143.10		NIST Webbook

Sources

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=U333834&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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