O-(4-Hydroxybenzoyl)tropine, O-methyl-

Inchi: InChI=1S/C16H21NO3/c1-17-12-5-6-13(17)10-15(9-12)20-16(18)11-3-7-14(19-2)8-4-11/h
InchiKey: JOROTINCCHPFDK-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: COc1ccc(C(=O)OC2CC3CCC(C2)N3C)cc1
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.477		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
rinpol	2323.00		NIST Webbook

Sources

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=U374670&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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