Benzeneacetic acid, «alpha»-hydroxy-, 1,2,2,6-tetramethyl-4-piperidinyl ester

Other names: Eucatropine
1,2,2,6-Tetramethyl-4-piperidyl mandelate
Euphthalmine

Inchi: InChI=1S/C17H25NO3/c1-12-10-14(11-17(2,3)18(12)4)21-16(20)15(19)13-8-6-5-7-9-13/h

InchiKey: QSAVEGSLJISCDF-UHFFFAOYSA-N

Formula: C17H25NO3

SMILES: CC1CC(OC(=O)C(O)c2ccccc2)CC(C)(C)N1C

Mol. weight [g/mol]: 291.39

CAS: 100-91-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.524		Crippen Method
mcvol	239.060	ml/mol	McGowan Method
rinpol	2026.00		NIST Webbook
rinpol	2026.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100914&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