

Benzeneacetic acid, «alpha»-hydroxy-, 1,2,2,6-tetramethyl-4-piperidinyI 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/

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.cheméo.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

Latest version available from:

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