EUCATROPINE

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.67		Cheméo Relay (1.0)
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices