Pellotine

Other names: Methylanhalonidine
Inchi: InChI=1S/C13H19NO3/c1-8-11-9(5-6-14(8)2)7-10(16-3)13(17-4)12(11)15/h7-8,15H,5-6H
InchiKey: NKHMWHLJHODBEP-UHFFFAOYSA-N
Formula: C13H19NO3
SMILES: COc1cc2c(c(O)c1OC)C(C)N(C)CC2
Mol. weight [g/mol]: 237.29
CAS: 83-14-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	1.958		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
rinpol	1800.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1800.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83147&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