

Pyrroliphene

Other names: (+)-«alpha»-Benzyl-«beta»-methyl-«alpha»-phenyl-1-pyrrolidinepropanol acetate (ester)
Pyrrolifene

Inchi: InChI=1S/C23H29NO2/c1-19(18-24-15-9-10-16-24)23(26-20(2)25,22-13-7-4-8-14-22)17-

InchiKey: XPSOFSIDLMRECY-UHFFFAOYSA-N

Formula: C23H29NO2

SMILES: CC(=O)OC(Cc1ccccc1)(c1ccccc1)C(C)CN1CCCC1

Mol. weight [g/mol]: 351.48

CAS: 15686-97-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	4.420		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C15686972&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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