1-Piperidinebutanol, alpha,alpha-diphenyl-, pamoate

Inchi: InChI=1S/C65H66N2O6/c68-60-56(54-35-17-15-25-48(54)45-58(60)62(70)72-64(50-27-7

InchiKey: XYQKJQBVPQOKHY-UHFFFAOYSA-N

Formula: C65H66N2O6

SMILES: O=C(OC(CCCN1CCCCC1)(c1ccccc1)c1ccccc1)c1cc2ccccc2c(Cc2c(O)c(C(=O)OC(CCC

Mol. weight [g/mol]: 971.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-17.39		Crippen Method
logp	13.728		Crippen Method
mcvol	770.090	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009832&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