1-(1-Pyrrolidinyl)-2,2-diphenyl-3-(phenylacetamido

Inchi: InChI=1S/C27H30N2O/c30-26(20-23-12-4-1-5-13-23)28-21-27(22-29-18-10-11-19-29,24
InchiKey: BZFXCKUBIBPKTI-UHFFFAOYSA-N
Formula: C27H30N2O
SMILES: O=C(Cc1ccccc1)NCC(CN1CCCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 398.54
CAS: 116595-10-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	4.427		Crippen Method
mcvol	330.680	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595109&Units=SI

Legend

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