1-(1-Pyrrolidinyl)-2,2-diphenyl-3-(acetamido)propa

Inchi: InChI=1S/C21H26N2O/c1-18(24)22-16-21(17-23-14-8-9-15-23,19-10-4-2-5-11-19)20-12-
InchiKey: ZBZVFNQNCXHPME-UHFFFAOYSA-N
Formula: C21H26N2O
SMILES: CC(=O)NCC(CN1CCCC1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 322.44
CAS: 116595-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	3.205		Crippen Method
mcvol	269.900	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595096&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