

1-(1-Pyrrolidiny1)-2,2-diphenyl-3-(acetamido)propane

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/ci9903071
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

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