N-benzoyl-a-1-piperidylbenzylamine

Inchi:	InChI=1S/C19H22N2O/c22-19(17-12-6-2-7-13-17)20-18(16-10-4-1-5-11-16)21-14-8-3-9-
InchiKey:	NVVFLNPPJPMLEF-UHFFFAOYSA-N
Formula:	C19H22N2O
SMILES:	OC(=NC(c1ccccc1)N1CCCCC1)c1ccccc1
Mol. weight [g/mol]:	294.39
CAS:	15563-53-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	4.176		Crippen Method
mcvol	241.720	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15563538&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

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