1-Benzoylpiperidine

Other names:	Piperidine, 1-benzoyl- «alpha»-Repellin Benzoic acid piperidide Benzoic acid N-piperidide Benzoylpiperidine LG 20104 N-Benzoyl piperidine N-Benzoylpiperidin P 162 Protectine I R 162 NSC 1992 NSC 26344
Inchi:	InChI=1S/C12H15NO/c14-12(11-7-3-1-4-8-11)13-9-5-2-6-10-13/h1,3-4,7-8H,2,5-6,9-10H
InchiKey:	YXTROGRGRSPWKL-UHFFFAOYSA-N
Formula:	C12H15NO
SMILES:	O=C(c1ccccc1)N1CCCCC1
Mol. weight [g/mol]:	189.25
CAS:	776-75-0

Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.313		Crippen Method
mcvol	156.870	ml/mol	McGowan Method
tb	593.70	K	NIST Webbook

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=C776750&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature