Phenol, m-(1-methyl-3-propyl-3-pyrrolidinyl)-

Other names:	CI 572
	Profadol
	A-2205
	3-(m-Hydroxyphenyl)-1-methyl-3-propylpyrrolidine
	Pyrrolidine, 3-(m-hydroxyphenyl)-1-methyl-3-propyl-
	m-(1-Methyl-3-propyl-3-pyrrolidinyl)phenol
Inchi:	InChI=1S/C14H21NO/c1-3-7-14(8-9-15(2)11-14)12-5-4-6-13(16)10-12/h4-6,10,16H,3,7-9
InchiKey:	VFUGCQKESINERB-UHFFFAOYSA-N
Formula:	C14H21NO
SMILES:	CCCC1(c2cccc(O)c2)CCN(C)C1
Mol. weight [g/mol]:	219.32
CAS:	428-37-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	2.766		Crippen Method
mcvol	189.350	ml/mol	McGowan Method
rinpol	1748.00		NIST Webbook
rinpol	1748.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C428375&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
rinpol:	Non-polar retention indices