

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/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
rinpol: Non-polar retention indices

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