

3-Pentyn-2-ol, 2-methyl-5-phenoxy-

Inchi:	InChI=1S/C12H14O2/c1-12(2,13)9-6-10-14-11-7-4-3-5-8-11/h3-5,7-8,13H,10H2,1-2H3
InchiKey:	YQBNDHADCCFJJQ-UHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	CC(C)([O])C#CCOc1ccccc1
Mol. weight [g/mol]:	190.24
CAS:	16488-98-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.48		Crippen Method
logp	2.278		Crippen Method
mcvol	157.170	ml/mol	McGowan Method

Sources

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=C16488985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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