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