1-Pentanol, 3-methyl-2-phenyl-

Inchi: InChI=1S/C12H18O/c1-3-10(2)12(9-13)11-7-5-4-6-8-11/h4-8,10,12-13H,3,9H2,1-2H3
InchiKey: BPCBJIKKAINGQY-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CCC(C)C(C[O])c1ccccc1
Mol. weight [g/mol]: 178.27
CAS: 36748-84-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.56		Crippen Method
logp	3.247		Crippen Method
mcvol	159.900	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36748842&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