

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/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

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<https://www.chemeo.com/cid/75-482-4/1-Pentanol-3-methyl-2-phenyl.pdf>

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