

1-(2-Furyl)-3-phenylpropane

Other names:	2-(3-Phenylpropyl)furan Furan, 2-(3-phenylpropyl)-
Inchi:	InChI=1S/C13H14O/c1-2-6-12(7-3-1)8-4-9-13-10-5-11-14-13/h1-3,5-7,10-11H,4,8-9H2
InchiKey:	HWYJSJWNOAJXLT-UHFFFAOYSA-N
Formula:	C13H14O
SMILES:	<chem>c1ccc(CCCc2ccco2)cc1</chem>
Mol. weight [g/mol]:	186.25
CAS:	5073-13-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	3.455		Crippen Method
mcvol	156.680	ml/mol	McGowan Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5073132&Units=SI

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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