

2-Furancarboxylic acid, 2-phenylethyl ester

Other names:	2-Furoic acid, phenethyl ester AI3-36016 Phenethyl 2-furoate 2-Furanecarboxylic acid, 2-phenylethyl ester 2-Phenylethyl 2-furoate
Inchi:	InChI=1S/C13H12O3/c14-13(12-7-4-9-15-12)16-10-8-11-5-2-1-3-6-11/h1-7,9H,8,10H2
InchiKey:	QKPSYARWSBJEDY-UHFFFAOYSA-N
Formula:	C13H12O3
SMILES:	O=C(OCCc1ccccc1)c1ccco1
Mol. weight [g/mol]:	216.23
CAS:	7149-32-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.48		Crippen Method
logp	2.679		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
rinsol	1760.00		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=C7149328&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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