1-phenyl-2-(2-furanyl)-ethane

Inchi: InChI=1S/C12H12O/c1-2-5-11(6-3-1)8-9-12-7-4-10-13-12/h1-7,10H,8-9H2
InchiKey: PPRMBHRATOCDLN-UHFFFAOYSA-N
Formula: C12H12O
SMILES: c1ccc(CCc2ccco2)cc1
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.62		Crippen Method
logp	3.065		Crippen Method
mcvol	142.590	ml/mol	McGowan Method
ripol	1858.00		NIST Webbook
ripol	1858.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R492801&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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