2-pentenylfuran

Inchi: InChI=1S/C9H12O/c1-2-3-4-6-9-7-5-8-10-9/h4-8H,2-3H2,1H3/b6-4+
InchiKey: LKSYSJTUBQSZBS-GQCTYLIASA-N
Formula: C9H12O
SMILES: CCCC=Cc1ccco1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.28		Crippen Method
logp	3.093		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
ripol	1297.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1297.00		NIST Webbook

Sources

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=R301394&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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