2-methyl-5-propenylfuran

Inchi: InChI=1S/C8H10O/c1-3-4-8-6-5-7(2)9-8/h3-6H,1-2H3/b4-3+
InchiKey: QXSXKNKKQRKGJB-ONEGZZNKSA-N
Formula: C8H10O
SMILES: CC=Cc1ccc(C)o1
Mol. weight [g/mol]: 122.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.92		Crippen Method
logp	2.621		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	972.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1262.00		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=R236616&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
ripol: Polar retention indices

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