2-ethyl-5-vinylfuran

Inchi: InChI=1S/C8H10O/c1-3-7-5-6-8(4-2)9-7/h3,5-6H,1,4H2,2H3
InchiKey: IXUQNBIJEOYXFG-UHFFFAOYSA-N
Formula: C8H10O
SMILES: C=Cc1ccc(CC)o1
Mol. weight [g/mol]: 122.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.83		Crippen Method
logp	2.485		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
ripol	1209.00		NIST Webbook
ripol	1209.00		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=R301141&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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