

(E)-2-(1-Butenyl)furan

Inchi:	InChI=1S/C8H10O/c1-2-3-5-8-6-4-7-9-8/h3-7H,2H2,1H3/b5-3+
InchiKey:	UUSUYFDXZRCICK-HWKANZROSA-N
Formula:	C8H10O
SMILES:	CCC=Cc1ccco1
Mol. weight [g/mol]:	122.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.87		Crippen Method
logp	2.703		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	920.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R413135&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/25-670-0/E-2-1-Butenyl-furan.pdf>

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