

2-propenylfuran

Other names: 2-(1-propenyl)furan
Inchi: InChI=1S/C7H8O/c1-2-4-7-5-3-6-8-7/h2-6H,1H3/b4-2+
InchiKey: IGWQTPINFQSICW-DUXPYHPUSA-N
Formula: C7H8O
SMILES: CC=Cc1ccco1
Mol. weight [g/mol]: 108.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Crippen Method
logp	2.313		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
ripol	1184.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1196.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1183.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R301121&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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