

Furan, 2-(2-propenyl)-

Other names:	2-Allylfuran 2-(2-propenyl)furan
Inchi:	InChI=1S/C7H8O/c1-2-4-7-5-3-6-8-7/h2-3,5-6H,1,4H2
InchiKey:	ZNCOUMAUNDFVCZ-UHFFFAOYSA-N
Formula:	C7H8O
SMILES:	C=CCc1ccco1
Mol. weight [g/mol]:	108.14
CAS:	75135-41-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	2.008		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
rinpol	857.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	862.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1226.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75135410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ripol:	Polar retention indices

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