

2-Furancarboxylic acid, 2-propenyl ester

Other names:	2-Furoic acid, allyl ester Allyl 2-furoate Allyl 2-furancarboxylate 2-Furancarboxylic acid, allyl ester Allyl furoate
Inchi:	InChI=1S/C8H8O3/c1-2-5-11-8(9)7-4-3-6-10-7/h2-4,6H,1,5H2
InchiKey:	SJRQTHAMRUOPBJ-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	C=CCOC(=O)c1ccco1
Mol. weight [g/mol]:	152.15
CAS:	4208-49-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.14		Crippen Method
logp	1.622		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
rinpol	1113.00		NIST Webbook
rinpol	1113.00		NIST Webbook
ripol	1748.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4208495&Units=SI
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

Legend

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

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