

2-Propenoic acid, 3-(2-furanyl)-, 2-methylpropyl ester

Other names:	iso-Butyl «beta»-2-furyl-acrylate Isobutyl 3-(2-furyl)-2-propenoate Isobutyl 3-(2-furyl)acrylate Isobutyl 2-furylacrylate
Inchi:	InChI=1S/C11H14O3/c1-9(2)8-14-11(12)6-5-10-4-3-7-13-10/h3-7,9H,8H2,1-2H3/b6-5+
InchiKey:	MXZZSWRRDGWLK-AATRIKPKSA-N
Formula:	C11H14O3
SMILES:	CC(C)COC(=O)C=Cc1ccco1
Mol. weight [g/mol]:	194.23
CAS:	68480-18-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.74		Crippen Method
logp	2.492		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
rinpol	1435.00		NIST Webbook
ripol	2006.00		NIST Webbook

Sources

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=C68480182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.cheméo.com/cid/62-282-0/2-Propenoic-acid-3-2-furanyl-2-methylpropyl-ester.pdf>

Generated by Cheméo on 2025-12-05 20:07:56.768197162 +0000 UTC m=+4713474.298237826.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.