

# 2-[(methylthio)methyl]-3-(2-furyl)acrolein (cis- or trans-)

Other names:	2-[(methylthio)methyl]-3-(2-furyl)acrolein
Inchi:	InChI=1S/C9H10O2S/c1-12-7-8(6-10)5-9-3-2-4-11-9/h2-6H,7H2,1H3/b8-5-
InchiKey:	UZAOTKQAYJZKLG-YVMONPNESA-N
Formula:	C9H10O2S
SMILES:	CSCC(C=O)=Cc1ccco1
Mol. weight [g/mol]:	182.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Crippen Method
logp	2.225		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
rinsol	1456.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U366021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U366021&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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