

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

Other names:	2-[(methylthio)methyl]-3-(3-furyl)acrolein
Inchi:	InChI=1S/C9H10O2S/c1-12-7-9(5-10)4-8-2-3-11-6-8/h2-6H,7H2,1H3/b9-4+
InchiKey:	ZHAZDGZQQKMJBO-RUDMXATFSA-N
Formula:	C9H10O2S
SMILES:	CSCC(C=O)=Cc1ccoc1
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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U366007&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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