

Dimethenamid

Other names:	Acetamide, 2-chloro-N-(2,4-dimethyl-3-thienyl)-N-(2-methoxy-1-methylethyl)-
Inchi:	InChI=1S/C12H18ClNO2S/c1-8-7-17-10(3)12(8)14(11(15)5-13)9(2)6-16-4/h7,9H,5-6H2,1
InchiKey:	JLYFCTQDENRSOL-UHFFFAOYSA-N
Formula:	C12H18ClNO2S
SMILES:	COCC(C)N(C(=O)CCl)c1c(C)csc1C
Mol. weight [g/mol]:	275.80
CAS:	87674-68-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	2.972		Crippen Method
mcvol	206.490	ml/mol	McGowan Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87674688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/85-713-6/Dimethenamid.pdf>

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