

Thenylchlor

Other names:	Acetamide, 2-chloro-N-(2,6-dimethylphenyl)-N-[(3-methoxy-2-thienyl)methyl]-
Inchi:	InChI=1S/C16H18ClNO2S/c1-11-5-4-6-12(2)16(11)18(15(19)9-17)10-14-13(20-3)7-8-21-
InchiKey:	KDWQYMVPYJGPHS-UHFFFAOYSA-N
Formula:	C16H18ClNO2S
SMILES:	COc1ccsc1CN(C(=O)CCl)c1c(C)cccc1C
Mol. weight [g/mol]:	323.84
CAS:	96491-05-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.66		Crippen Method
logp	4.146		Crippen Method
mcvol	239.090	ml/mol	McGowan Method
rinpol	2367.00		NIST Webbook
rinpol	2384.00		NIST Webbook
rinpol	2367.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96491053&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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