

2,3,3-Trichloro-n-(2-thiazole) acrylamide

Inchi:	InChI=1S/C6H3Cl3N2OS/c7-3(4(8)9)5(12)11-6-10-1-2-13-6/h1-2H,(H,10,11,12)
InchiKey:	ZCWOFZLPIRURHO-UHFFFAOYSA-N
Formula:	C6H3Cl3N2OS
SMILES:	O=C(Nc1nccs1)C(Cl)=C(Cl)Cl
Mol. weight [g/mol]:	257.52
CAS:	99516-00-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	2.967		Crippen Method
mcvol	146.240	ml/mol	McGowan Method

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=C99516004&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

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<https://www.chemeo.com/cid/118-456-5/2-3-3-Trichloro-n-2-thiazole-acrylamide.pdf>

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