

N,n'-diacetyl-n,n'-bis-[5-chloro-1,3,4-thiadiazolyl]-2

Inchi:	InChI=1S/C8H6Cl2N6O2S2/c1-3(17)15(7-13-11-5(9)19-7)16(4(2)18)8-14-12-6(10)20-8/h
InchiKey:	IUMJNTAJYBUFGP-UHFFFAOYSA-N
Formula:	C8H6Cl2N6O2S2
SMILES:	CC(=O)N(c1nnc(Cl)s1)N(C(C)=O)c1nnc(Cl)s1
Mol. weight [g/mol]:	353.21
CAS:	100191-60-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.017		Crippen Method
mcvol	204.860	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=C100191604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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