

3,4-Diacetyl-5-thione-1,3,4-thiadiazolidone-2-azine

Inchi:	InChI=1S/C12H12N6O4S4/c1-5(19)15-9(25-11(23)17(15)7(3)21)13-14-10-16(6(2)20)18(
InchiKey:	WGYBHZHVQMMWAX-ZKLMZBBOSA-N
Formula:	C12H12N6O4S4
SMILES:	CC(=O)n1c(=S)sc(=NN=c2sc(=S)n(C(C)=O)n2C(C)=O)n1C(C)=O
Mol. weight [g/mol]:	432.52
CAS:	108040-17-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	1.532		Crippen Method
mcvol	272.580	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108040171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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