

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

Inchi:	InChI=1S/C12H12N6O6S2/c1-5(19)15-9(25-11(23)17(15)7(3)21)13-14-10-16(6(2)20)18(
InchiKey:	WMZQYICDOSNCIN-ZKLMZBBOSA-N
Formula:	C12H12N6O6S2
SMILES:	CC(=O)n1c(=O)sc(=NN=c2sc(=O)n(C(C)=O)n2C(C)=O)n1C(C)=O
Mol. weight [g/mol]:	400.39
CAS:	108952-44-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	-1.207		Crippen Method
mcvol	251.620	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108952449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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