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(8

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/ci990307l

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