4,4'-Diacetyl-[2,2'-azo-1,3,4-thiadiazol-5-one]

Inchi: InChI=1S/C8H6N6O4S2/c1-3(15)13-7(17)19-5(11-13)9-10-6-12-14(4(2)16)8(18)20-6/h1-
InchiKey: WEVDGPZETOVFSR-MDZDMXLPSA-N
Formula: C8H6N6O4S2
SMILES: CC(=O)n1nc(N=Nc2nn(C(C)=O)c(=O)s2)sc1=O
Mol. weight [g/mol]: 314.30
CAS: 116529-22-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	0.659		Crippen Method
mcvol	187.820	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116529227&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