Rhodanine, n-diacetylamino-

Inchi: InChI=1S/C7H8N2O3S2/c1-4(10)8(5(2)11)9-6(12)3-14-7(9)13/h3H2,1-2H3
InchiKey: QASDIQBQSQLCHF-UHFFFAOYSA-N
Formula: C7H8N2O3S2
SMILES: CC(=O)N(C(C)=O)N1C(=O)CSC1=S
Mol. weight [g/mol]: 232.28
CAS: 20904-81-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	0.157		Crippen Method
mcvol	151.700	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=C20904818&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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