2,6-Diacetoacetamidopyridine

Inchi: InChI=1S/C13H15N3O4/c1-8(17)6-12(19)15-10-4-3-5-11(14-10)16-13(20)7-9(2)18/h3-5H
InchiKey: DHZQCPZPEGHVNI-UHFFFAOYSA-N
Formula: C13H15N3O4
SMILES: CC(=O)CC(=O)Nc1cccc(NC(=O)CC(C)=O)n1
Mol. weight [g/mol]: 277.28
CAS: 63896-86-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	0.917		Crippen Method
mcvol	206.490	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C63896866&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