

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

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