

Pyrrolidine, n-[2,6-dioxo-4-piperidiny]acetyl]-

Inchi:	InChI=1S/C11H16N2O3/c14-9-5-8(6-10(15)12-9)7-11(16)13-3-1-2-4-13/h8H,1-7H2,(H,12)
InchiKey:	DZDYTSKLBQZULC-UHFFFAOYSA-N
Formula:	C11H16N2O3
SMILES:	O=C1CC(CC(=O)N2CCCC2)CC(=O)N1
Mol. weight [g/mol]:	224.26
CAS:	6939-31-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	0.052		Crippen Method
mcvol	168.800	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6939317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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