

Acetamide, n-(6-formyl-4-oxo-(3h)-pyrimidin-2-yl)-

Inchi:	InChI=1S/C7H7N3O3/c1-4(12)8-7-9-5(3-11)2-6(13)10-7/h2-3H,1H3,(H2,8,9,10,12,13)
InchiKey:	ALKKEDWNQXAYHK-UHFFFAOYSA-N
Formula:	C7H7N3O3
SMILES:	CC(=O)Nc1nc(C=O)cc(=O)[nH]1
Mol. weight [g/mol]:	181.15
CAS:	60656-63-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	-0.941		Crippen Method
mcvol	124.680	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60656635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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