

2H-Pyrido[3,2-b]-1,4-oxazin-3(4H)-one

Inchi:	InChI=1S/C7H6N2O2/c10-6-4-11-5-2-1-3-8-7(5)9-6/h1-3H,4H2,(H,8,9,10)
InchiKey:	ANHQLUBMNSSPBV-UHFFFAOYSA-N
Formula:	C7H6N2O2
SMILES:	O=C1COc2cccnc2N1
Mol. weight [g/mol]:	150.13
CAS:	20348-09-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Crippen Method
logp	0.412		Crippen Method
mcvol	102.270	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20348098&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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