4H-Pyrido[1,2-a]pyrimidin-4-one, 2-methyl-

Inchi:	InChI=1S/C9H8N2O/c1-7-6-9(12)11-5-3-2-4-8(11)10-7/h2-6H,1H3
InchiKey:	UUXFTJCUPHVPKZ-UHFFFAOYSA-N
Formula:	C9H8N2O
SMILES:	Cc1cc(=O)n2ccccc2n1
Mol. weight [g/mol]:	160.17
CAS:	1693-94-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	1.003		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
rinpol	1648.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1693943&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
rinpol:	Non-polar retention indices

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