

4H-Pyrido[1,2-a]pyrimidin-4-one, 6,7,8,9-tetrahydro-6-methyl-

Other names:	MZ 132 6,7,8,9-Tetrahydro-6-methyl-4H-pyrido(1,2-a)pyrimidine-4-one 6-Methyl-6,7,8,9-tetrahydro-4H-pyrido[1,2-a]pyrimidin-4-one
Inchi:	InChI=1S/C9H12N2O/c1-7-3-2-4-8-10-6-5-9(12)11(7)8/h5-7H,2-4H2,1H3
InchiKey:	HCJOGZBBWGQKGC-UHFFFAOYSA-N
Formula:	C9H12N2O
SMILES:	CC1CCCc2nccc(=O)n21
Mol. weight [g/mol]:	164.20
CAS:	32092-29-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	1.141		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
rinpol	1578.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32092298&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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