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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices