

4H-Pyrido[1,2-a]pyrimidin-4-one, 3-methyl

Inchi: InChI=1S/C9H8N2O/c1-7-6-10-8-4-2-3-5-11(8)9(7)12/h2-6H,1H3
InchiKey: CVQGFKKCKVAEIK-UHFFFAOYSA-N
Formula: C9H8N2O
SMILES: Cc1cnc2ccccn2c1=O
Mol. weight [g/mol]: 160.17

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	1638.00		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=R64304&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

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<https://www.chemeo.com/cid/18-152-3/4H-Pyrido-1-2-a-pyrimidin-4-one-3-methyl.pdf>

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