

4H-Pyrido[1,2-a]pyrimidin-4-one, 3,6-dimethyl-

Other names: 3,6-Dimethyl-4H-pyrido[1,2-a]pyrimidin-4-one
3,6-Dimethyl-4H-pyrid-[1,2-a]-pyrimidin-4-one

Inchi: InChI=1S/C10H10N2O/c1-7-6-11-9-5-3-4-8(2)12(9)10(7)13/h3-6H,1-2H3

InchiKey: VNZAABOALQMGKL-UHFFFAOYSA-N

Formula: C10H10N2O

SMILES: Cc1cnc2cccc(C)n2c1=O

Mol. weight [g/mol]: 174.20

CAS: 39080-46-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.311		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
rinpol	1694.00		NIST Webbook
ripol	2144.00		NIST Webbook

Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C39080461&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices

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