

4H-Pyrido[1,2-a]pyrimidin-4-one, 2,9-dimethyl

Inchi: InChI=1S/C10H10N2O/c1-7-4-3-5-12-9(13)6-8(2)11-10(7)12/h3-6H,1-2H3
InchiKey: XXRSWHWERLUWQS-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: Cc1cc(=O)n2cccc(C)c2n1
Mol. weight [g/mol]: 174.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.311		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
rinpola	1714.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R119843&Units=SI>

Legend

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

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