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

Inchi: InChI=1S/C10H10N2O/c1-7-8(2)11-9-5-3-4-6-12(9)10(7)13/h3-6H,1-2H3
InchiKey: FXHOXXOPXPGPKP-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: Cc1nc2ccccn2c(=O)c1C
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
rinpol	1727.00		NIST Webbook
rinpol	1727.00		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=R119838&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

Latest version available from:
https://www.chemeo.com/cid/94-451-7/4H-Pyrido-1-2-a-pyrimidin-4-one-2-3-dimethyl.pdf
Generated by Cheméo on 2024-04-25 06:47:41.029519462 +0000 UTC m=+16316909.950096777.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.