4H-Pyrido[1,2-a]pyrimidin-4-one, 6,7,8,9-tetrahydro, 3-methyl

Inchi: InChI=1S/C9H12N2O/c1-7-6-10-8-4-2-3-5-11(8)9(7)12/h6H,2-5H2,1H3
InchiKey: BZOPBXXGKITYKL-UHFFFAOYSA-N
Formula: C9H12N2O
SMILES: Cc1cnc2n(c1=O)CCCC2
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	0.888		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64336&Units=SI
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

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/34-074-2/4H-Pyrido-1-2-a-pyrimidin-4-one-6-7-8-9-tetrahydro-3-methyl.pdf
Generated by Cheméo on 2024-10-12 04:55:55.3681929 +0000 UTC m=+3289818.005162149.

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