

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

InChI: Cc1nc2c(c1)ncnc2=O
InChIKey: ZXAUVBKRVIIVSX-UHFFFAOYSA-N
Formula: C₁₂H₁₂N₂O
SMILES: CC1CCc2cc3nccc(=O)n3cc21
Mol. weight [g/mol]: 200.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	1.744		Crippen Method
mcvol	151.690	ml/mol	McGowan Method
rinpol	1998.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R64215&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/58-249-2/4H-Cyclopenteno-2-3-e-pyrido-1-2-a-pyrimidin-4-one-6-7-8-9-tetrahydro-7-me>

Generated by Cheméo on 2024-04-24 21:55:28.114538111 +0000 UTC m=+16284977.035115422.

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