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

Inchi: InChI=1S/C9H12N2O/c1-7-3-2-6-11-8(12)4-5-10-9(7)11/h4-5,7H,2-3,6H2,1H3
InchiKey: RBJWQZWEWIGJDH-UHFFFAOYSA-N
Formula: C9H12N2O
SMILES: CC1CCCn2c1nccc2=O
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	1.141		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
rinpol	1615.00		NIST Webbook
rinpol	1615.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64368&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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