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

Inchi: InChI=1S/C9H12N2O/c1-7-6-9(12)11-5-3-2-4-8(11)10-7/h6H,2-5H2,1H3
InchiKey: WCVUTDNAIJJMSX-UHFFFAOYSA-N
Formula: C9H12N2O
SMILES: Cc1cc(=O)n2c(n1)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	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64322&Units=SI

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.