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

Inchi: InChI=1S/C9H12N2O/c1-7-3-5-11-8(6-7)10-4-2-9(11)12/h2,4,7H,3,5-6H2,1H3
InchiKey: HITNVWSZJDFAIF-UHFFFAOYSA-N
Formula: C9H12N2O
SMILES: CC1CCn2c(nccc2=O)C1
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	0.826		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
rinpol	1638.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64354&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