4H-Pyrido[1,2-a]pyrimidin-4-one

Inchi: InChI=1S/C8H6N2O/c11-8-4-5-9-7-3-1-2-6-10(7)8/h1-6H
InchiKey: NYJWYCAHJRGKMI-UHFFFAOYSA-N
Formula: C8H6N2O
SMILES: O=c1ccnc2ccccn12
Mol. weight [g/mol]: 146.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	0.694		Crippen Method
mcvol	106.190	ml/mol	McGowan Method
rinpol	1580.00		NIST Webbook
rinpol	1580.00		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=R64297&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.