1,2,3,4-Tetrahydropyrido-[1,2-a] benzimidazole

Inchi: InChI=1S/C11H12N2/c1-2-6-10-9(5-1)12-11-7-3-4-8-13(10)11/h1-2,5-6H,3-4,7-8H2
InchiKey: QHDDBWGHEWTMDV-UHFFFAOYSA-N
Formula: C11H12N2
SMILES: c1ccc2c(c1)nc1n2CCCC1
Mol. weight [g/mol]: 172.23
CAS: 5622-83-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	2.373		Crippen Method
mcvol	136.030	ml/mol	McGowan Method

Sources

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=C5622833&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume