

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

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