1H-pyrido[3,4-b]indole-3-carboxylic acid, 2,3,4,9-tetrahydro-

Inchi: InChI=1S/C12H12N2O2/c15-12(16)10-5-8-7-3-1-2-4-9(7)14-11(8)6-13-10/h1-4,10,13-14H

InchiKey: FSNCEEGOMTYXKY-UHFFFAOYSA-N

Formula: C12H12N2O2

SMILES: O=C([O-])C1Cc2c([nH]c3ccccc23)C[NH2+]1

Mol. weight [g/mol]: 216.24

CAS: 6052-68-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	-1.576		Crippen Method
mcvol	157.560	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=C6052682&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