

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
mvol	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/ci9903071

Legend

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

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