

Indole-1-propionic acid

Other names:	1H-indole-1-propionic acid
Inchi:	InChI=1S/C11H11NO2/c13-11(14)6-8-12-7-5-9-3-1-2-4-10(9)12/h1-5,7H,6,8H2,(H,13,14)
InchiKey:	OSWNOVFZARRSKM-UHFFFAOYSA-N
Formula:	C11H11NO2
SMILES:	O=C(O)CCn1ccc2ccccc21
Mol. weight [g/mol]:	189.21
CAS:	6639-06-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	2.116		Crippen Method
mcvol	144.350	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6639061&Units=SI

Legend

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

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