

Indole-3-pyruvic acid

Other names:	3-Indolepyruvic acid 1H-Indole-3-propanoic acid, «alpha»-oxo- Indole-3-pyruvate «beta»-Indolepyruvic acid 3-Indolylpyrrolic acid Indolyl-3-pyruvate «beta»-Indolylpyruvic acid 3-Indolylpyruvic acid 3-(1H-Indol-3-yl)-2-oxopropanoic acid 1H-Indole-3-pyruvic acid NSC 88874 indole-3-pyruvic acid monohydrate
Inchi:	InChI=1S/C11H9NO3/c13-10(11(14)15)5-7-6-12-9-4-2-1-3-8(7)9/h1-4,6,12H,5H2,(H,14,15)
InchiKey:	RSTKLPZEZYGQPY-UHFFFAOYSA-N
Formula:	C11H9NO3
SMILES:	O=C(O)C(=O)Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	203.19
CAS:	392-12-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	0.882		Crippen Method
mvol	145.920	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=C392121&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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