

1-Acetyl-5-iodoindoline

Inchi:	InChI=1S/C10H10INO/c1-7(13)12-5-4-8-6-9(11)2-3-10(8)12/h2-3,6H,4-5H2,1H3
InchiKey:	ATPPCQXBZHKNFO-UHFFFAOYSA-N
Formula:	C10H10INO
SMILES:	CC(=O)N1CCc2cc(I)ccc21
Mol. weight [g/mol]:	287.10
CAS:	61995-51-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	2.200		Crippen Method
mcvol	154.510	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61995515&Units=SI
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

Legend

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

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