5,6-Dimethoxyindole

Other names:	1H-Indole, 5,6-dimethoxy-
	5,6-dimethoxy-1H-indole
Inchi:	InChI=1S/C10H11NO2/c1-12-9-5-7-3-4-11-8(7)6-10(9)13-2/h3-6,11H,1-2H3
InchiKey:	QODBZRNBPUPLEZ-UHFFFAOYSA-N
Formula:	C10H11NO2
SMILES:	COc1cc2cc[nH]c2cc1OC
Mol. weight [g/mol]:	177.20
CAS:	14430-23-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.703		Crippen Method
mcvol	134.560	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=C14430230&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

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