5-Bromoindoxyl acetate

Other names:	o-Acetyl-5-bromoindoxyl
	1H-Indol-3-ol, 5-bromo-, acetate
	1H-Indol-3-ol, 5-bromo-, acetate (ester)
	5-Bromoindoxyl-3-acetate
	5-bromo-1H-indol-3-yl acetate
Inchi:	InChI=1S/C10H8BrNO2/c1-6(13)14-10-5-12-9-3-2-7(11)4-8(9)10/h2-5,12H,1H3
InchiKey:	KFTGECHXNQBTNZ-UHFFFAOYSA-N
Formula:	C10H8BrNO2
SMILES:	CC(=O)Oc1c[nH]c2ccc(Br)cc12
Mol. weight [g/mol]:	254.08
CAS:	17357-14-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	2.374		Crippen Method
mcvol	147.760	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17357141&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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