1H-Indol-3-ol, 1-acetyl-5-bromo-, acetate

Other names:	5-Bromoindoxyl diacetate
	5-Bromoindoxyl acetate
	1-Acetyl-5-bromo-1H-indol-3-yl acetate
	N-acetyl-5-bromoindolyl acetate
Inchi:	InChI=1S/C12H10BrNO3/c1-7(15)14-6-12(17-8(2)16)10-5-9(13)3-4-11(10)14/h3-6H,1-2H
InchiKey:	XJRIDJAGAYGJCK-UHFFFAOYSA-N
Formula:	C12H10BrNO3
SMILES:	CC(=O)Oc1cn(C(C)=O)c2ccc(Br)cc12
Mol. weight [g/mol]:	296.12
CAS:	33588-54-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	2.989		Crippen Method
mcvol	177.510	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33588544&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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