

3-Acetyl-6-bromocoumarin

Other names:	3-Acetyl-6-bromo-chromen-2-one
Inchi:	InChI=1S/C11H7BrO3/c1-6(13)9-5-7-4-8(12)2-3-10(7)15-11(9)14/h2-5H,1H3
InchiKey:	XFQYOFLFNKCHLG-UHFFFAOYSA-N
Formula:	C11H7BrO3
SMILES:	CC(=O)c1cc2cc(Br)ccc2oc1=O
Mol. weight [g/mol]:	267.07
CAS:	2199-93-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.26		Crippen Method
logp	2.758		Crippen Method
mcvol	153.440	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2199931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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