

3-Acetylamino coumarin

Other names:	3-Acetamidocoumarin
Inchi:	InChI=1S/C11H9NO3/c1-7(13)12-9-6-8-4-2-3-5-10(8)15-11(9)14/h2-6H,1H3,(H,12,13)
InchiKey:	XJYLCCJIDYSFMB-UHFFFAOYSA-N
Formula:	C11H9NO3
SMILES:	CC(=O)Nc1cc2ccccc2oc1=O
Mol. weight [g/mol]:	203.19
CAS:	779-30-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.63		Crippen Method
logp	1.751		Crippen Method
mcvol	145.920	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=C779306&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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