

# 7-Amino-4-(methoxymethyl)coumarin

<b>Inchi:</b>	InChI=1S/C11H11NO3/c1-14-6-7-4-11(13)15-10-5-8(12)2-3-9(7)10/h2-5H,6,12H2,1H3
<b>InchiKey:</b>	QZZLLHOMMCKWIQ-UHFFFAOYSA-N
<b>Formula:</b>	C11H11NO3
<b>SMILES:</b>	COCc1cc(=O)oc2cc(N)ccc12
<b>Mol. weight [g/mol]:</b>	205.21
<b>CAS:</b>	175205-10-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Crippen Method
logp	1.522		Crippen Method
mcvol	150.220	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C175205104&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C175205104&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/44-509-8/7-Amino-4-methoxymethyl-coumarin.pdf>

Generated by Cheméo on 2024-04-27 02:39:35.34038089 +0000 UTC m=+16474824.260958205.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.