

# 4H-Cyclopenta[b]thiophene-3-carboxylic acid, 2-amino-5,6-dihydro-, ethyl ester

<b>Other names:</b>	2-Amino-cyclopentano-[b]-thiophen-3-carboxylic acid, 5,6-dihydro-, ethyl ester 2-Amino-5,6-dihydro-4H-cyclopenta[b]thiophene-3-carboxylic acid ethyl ester
<b>Inchi:</b>	InChI=1S/C10H13NO2S/c1-2-13-10(12)8-6-4-3-5-7(6)14-9(8)11/h2-5,11H2,1H3
<b>InchiKey:</b>	BOJXCJDYZJSPMZ-UHFFFAOYSA-N
<b>Formula:</b>	C10H13NO2S
<b>SMILES:</b>	CCOC(=O)c1c(N)sc2c1CCC2
<b>Mol. weight [g/mol]:</b>	211.28
<b>CAS:</b>	4815-29-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.996		Crippen Method
mcvol	155.210	ml/mol	McGowan Method
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4815296&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4815296&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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
<b>rinpol:</b>	Non-polar retention indices

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