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

Other names: 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

Inchi: InChI=1S/C10H13NO2S/c1-2-13-10(12)8-6-4-3-5-7(6)14-9(8)11/h2-5,11H2,1H3

InchiKey: BOJXCJDYZJSPMZ-UHFFFAOYSA-N

Formula: C10H13NO2S

SMILES: CCOC(=O)c1c(N)sc2c1CCC2

Mol. weight [g/mol]: 211.28

CAS: 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4815296&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

rinpol: Non-polar retention indices