

«beta»-Alanine, N-(thiophene-2-carbonyl)-, ethyl ester

Inchi:	InChI=1S/C10H13NO3S/c1-2-14-9(12)5-6-11-10(13)8-4-3-7-15-8/h3-4,7H,2,5-6H2,1H3,(
InchiKey:	CHUSYYGICOPRMO-UHFFFAOYSA-N
Formula:	C10H13NO3S
SMILES:	CCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	227.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	1.431		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
rinsol	1917.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321793&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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