

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

Inchi:	InChI=1S/C12H17NO3S/c1-2-3-8-16-11(14)6-7-13-12(15)10-5-4-9-17-10/h4-5,9H,2-3,6-8
InchiKey:	UIDZMYUGPOKBEQ-UHFFFAOYSA-N
Formula:	C12H17NO3S
SMILES:	CCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	255.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	2.211		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321795&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321795&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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