

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

Inchi: InChI=1S/C19H31NO3S/c1-2-3-4-5-6-7-8-9-10-15-23-18(21)13-14-20-19(22)17-12-11-16
InchiKey: PPNHLIUUVWDYZDF-UHFFFAOYSA-N
Formula: C19H31NO3S
SMILES: CCCCCCCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]: 353.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	4.942		Crippen Method
mcvol	294.450	ml/mol	McGowan Method
rinpol	2889.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321802&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/43-654-8/beta-Alanine-N-thiophene-2-carbonyl-undecyl-ester.pdf>

Generated by Cheméo on 2025-12-25 00:41:58.339498774 +0000 UTC m=+6371515.869539429.

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