

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

**Inchi:** InChI=1S/C17H27NO3S/c1-2-3-4-5-6-7-8-13-21-16(19)11-12-18-17(20)15-10-9-14-22-15  
**InchiKey:** DIYJZQYVSLXPKI-UHFFFAOYSA-N  
**Formula:** C17H27NO3S  
**SMILES:** CCCCCCCCCOC(=O)CCNC(=O)c1cccs1  
**Mol. weight [g/mol]:** 325.47

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.04   |        | Crippen Method |
| logp          | 4.162   |        | Crippen Method |
| mcvol         | 266.270 | ml/mol | McGowan Method |
| rinpola       | 2641.00 |        | NIST Webbook   |
| rinpola       | 2641.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321800&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

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