

«beta»-Alanine, N-(2-furoyl)-, hexadecyl ester

Inchi: InChI=1S/C24H41NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-29-23(26)18-19-25-24(27)
InchiKey: IIHOTSMHQPEAHK-UHFFFAOYSA-N
Formula: C₂₄H₄₁NO₄
SMILES: CCCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 407.59

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -11.95 | | Crippen Method |
| logp | 6.424 | | Crippen Method |
| mcvol | 354.420 | ml/mol | McGowan Method |
| rinpol | 3415.00 | | NIST Webbook |
| rinpol | 3415.00 | | 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=U321985&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

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