

L-Alanine, N-[N-[N-(1-oxodecyl)glycyl]-L-tryptophyl]-L-alanine methyl ester

Other names: Alanine, N-[N-[N-(N-decanoyl)glycyl]-L-tryptophyl]-L-alanyl-, methyl ester, L-

Inchi: InChI=1S/C30H45N5O6/c1-5-6-7-8-9-10-11-16-26(36)32-19-27(37)35-25(17-22-18-31-24)

InchiKey: MPMCVDLITHVKGR-UHFFFAOYSA-N

Formula: C30H45N5O6

SMILES: CCCCCCCCCC(=O)NCC(=O)NC(Cc1c[nH]c2ccccc12)C(=O)NC(C)C(=O)NC(C)C(=O)O

Mol. weight [g/mol]: 571.71

CAS: 19716-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	2.153		Crippen Method
mcvol	458.260	ml/mol	McGowan Method

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=C19716780&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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