

D-Tryptophan, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi:	InChI=1S/C22H30N2O6/c1-6-28-21(26)23-18(20(25)30-15(5)14(3)4)12-16-13-24(22(27)28)
InchiKey:	IJUBFADZGYKUJR-NNJIEVJOSA-N
Formula:	C22H30N2O6
SMILES:	CCOC(=O)NC(Cc1cn(C(=O)OCC)c2ccccc12)C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	418.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	3.891		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
rinpola	2656.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R501965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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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