d-Proline, N-methoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C19H35NO4/c1-3-4-5-6-7-8-9-10-11-12-16-24-18(21)17-14-13-15-20(17)19(22
InchiKey: ODCNMSIMSUSGQH-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OC
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	4.681		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
rinpol	2317.00		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=U320795&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