

d-Proline, N-allyloxycarbonyl-, decyl ester

Inchi: InChI=1S/C19H33NO4/c1-3-5-6-7-8-9-10-11-16-23-18(21)17-13-12-14-20(17)19(22)24-1
InchiKey: OLJMBPQLESIYAK-UHFFFAOYSA-N
Formula: C19H33NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 339.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	4.457		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320970&Units=SI>
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>

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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