D-Proline, N-allyloxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C21H37NO4/c1-3-5-6-7-8-9-10-11-12-13-18-25-20(23)19-15-14-16-22(19)21(2
InchiKey: WZVNNRMSQUXSNZ-UHFFFAOYSA-N
Formula: C21H37NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 367.53

Physical Properties

Property code	Value	Unit	Source
logp	5.238		Crippen Method
mcvol	316.450	ml/mol	McGowan Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	662.77	K	Cheméo Relay (1.0)
tf	296.27	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320972&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point