

D-Proline, N-allyloxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C23H41NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-20-27-22(25)21-17-16-18-24(2)
InchiKey: HWCJKUPEVGYCPE-UHFFFAOYSA-N
Formula: C23H41NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 395.58

Physical Properties

Property code	Value	Unit	Source
logp	6.018		Crippen Method
mcvol	344.630	ml/mol	McGowan Method
rinpol	2842.00		NIST Webbook
rinpol	2842.00		NIST Webbook
tb	676.12	K	Cheméo Relay (1.0)
tf	303.47	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320973&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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

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