D-Proline, N-propoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C18H33NO4/c1-3-5-6-7-8-9-10-15-22-17(20)16-12-11-13-19(16)18(21)23-14-4
InchiKey: SFLZKSXXQIXQEI-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
logp	4.291		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tf	286.81	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320826&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
tf: Normal melting (fusion) point