D-Proline, N-methoxycarbonyl-, octyl ester

Inchi: InChI=1S/C15H27NO4/c1-3-4-5-6-7-8-12-20-14(17)13-10-9-11-16(13)15(18)19-2/h13H,3
InchiKey: REUVCMRMMIIVEL-UHFFFAOYSA-N
Formula: C15H27NO4
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)OC
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
logp	3.121		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	1967.00		NIST Webbook
tf	304.20	K	Cheméo Relay (1.0)

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320792&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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