D-Proline, N-propoxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C27H51NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-31-26(29)25-2
InchiKey: AORYCEYEWUIFDG-UHFFFAOYSA-N
Formula: C27H51NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]: 453.71

Physical Properties

Property code	Value	Unit	Source
logp	7.802		Crippen Method
mcvol	405.290	ml/mol	McGowan Method
rinpol	3081.00		NIST Webbook
rinpol	3081.00		NIST Webbook
tf	318.25	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320833&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

Legend

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

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