D-Proline, N-ethoxycabonyl-, undecyl ester

Inchi: InChI=1S/C19H35NO4/c1-3-5-6-7-8-9-10-11-12-16-24-18(21)17-14-13-15-20(17)19(22)2
InchiKey: NPPXNOFPQDCHOH-UHFFFAOYSA-N
Formula: C19H35NO4
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 341.49

Physical Properties

Property code	Value	Unit	Source
hvap	105.91	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.61		Cheméo Relay (1.0)
logp	4.681		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	629.08	K	Cheméo Relay (1.0)
tf	298.23	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=U320842&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
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