D-Proline, N-ethoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C22H41NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-19-27-21(24)20-17-16-18-23(2
InchiKey: RNMNESBBHQMAGA-UHFFFAOYSA-N
Formula: C22H41NO4
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 383.57

Physical Properties

Property code	Value	Unit	Source
hvap	117.79	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.52		Cheméo Relay (1.0)
logp	5.852		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
rinpol	2527.00		NIST Webbook
tb	648.78	K	Cheméo Relay (1.0)
tf	309.74	K	Cheméo Relay (1.0)

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320844&Units=SI

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