D-Proline, N-ethoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C25H47NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-30-24(27)23-20-1
InchiKey: KTTBCKAXKPKGMD-UHFFFAOYSA-N
Formula: C25H47NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 425.65

Physical Properties

Property code	Value	Unit	Source
hvap	129.59	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.46		Cheméo Relay (1.0)
logp	7.022		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpol	2816.00		NIST Webbook
tb	668.01	K	Cheméo Relay (1.0)
tf	318.29	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=U320847&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