D-Proline, N-butoxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C25H47NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-22-29-24(27)23-19-18-20-

InchiKey: OIVSUNLPDDRBLD-UHFFFAOYSA-N

Formula: C25H47NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCCC

Mol. weight [g/mol]: 425.65

Physical Properties

Property code	Value	Unit	Source
hvap	125.65	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.29		Cheméo Relay (1.0)
logp	7.022		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	668.03	K	Cheméo Relay (1.0)
tf	307.73	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=U321092&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

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