D-Proline, N-butoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-23-30-25(28)24-20-19-
InchiKey: RRXGBPBVZRDSHC-UHFFFAOYSA-N
Formula: C26H49NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCCC
Mol. weight [g/mol]: 439.68

Physical Properties

Property code	Value	Unit	Source
hvap	129.53	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.61		Cheméo Relay (1.0)
logp	7.412		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook
tb	674.41	K	Cheméo Relay (1.0)
tf	310.59	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321093&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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