D-Proline, N-butoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C17H31NO4/c1-3-5-7-8-9-14-21-16(19)15-11-10-12-18(15)17(20)22-13-6-4-2/h
InchiKey: APETUAKJTJTKOY-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)OCCCC
Mol. weight [g/mol]: 313.44

Physical Properties

Property code	Value	Unit	Source
hvap	94.71	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.74		Cheméo Relay (1.0)
logp	3.901		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
tb	614.81	K	Cheméo Relay (1.0)
tf	275.63	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=U321085&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
tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point