D-proline, n-ethoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C24H45NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-21-29-23(26)22-19-18-2
InchiKey: DGQMEPYDCCUTCA-UHFFFAOYSA-N
Formula: C24H45NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 411.63

Physical Properties

Property code	Value	Unit	Source
hvap	125.67	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.14		Cheméo Relay (1.0)
logp	6.632		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
tb	661.61	K	Cheméo Relay (1.0)
tf	316.05	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=U320846&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