D-Proline, N-ethoxycarbonyl-, hexyl ester

Inchi: InChI=1S/C14H25NO4/c1-3-5-6-7-11-19-13(16)12-9-8-10-15(12)14(17)18-4-2/h12H,3-11
InchiKey: QOTDAKXXZNZNFC-UHFFFAOYSA-N
Formula: C14H25NO4
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 271.36

Physical Properties

Property code	Value	Unit	Source
hvap	86.87	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.76		Cheméo Relay (1.0)
logp	2.731		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1822.00		NIST Webbook
tb	592.06	K	Cheméo Relay (1.0)
tf	276.89	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320837&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):

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