D-Proline, N-ethoxycarbonyl-, octyl ester

Inchi: InChI=1S/C16H29NO4/c1-3-5-6-7-8-9-13-21-15(18)14-11-10-12-17(14)16(19)20-4-2/h14
InchiKey: AFUJGVPDEKDTQZ-UHFFFAOYSA-N
Formula: C16H29NO4
SMILES: CCCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
hvap	95.12	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.56		Cheméo Relay (1.0)
logp	3.511		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpol	2010.00		NIST Webbook
tb	607.59	K	Cheméo Relay (1.0)
tf	279.95	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320839&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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