D-Proline, N-ethoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C15H27NO4/c1-3-5-6-7-8-12-20-14(17)13-10-9-11-16(13)15(18)19-4-2/h13H,3
InchiKey: FCZWAVXNQCLKMV-UHFFFAOYSA-N
Formula: C15H27NO4
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
hvap	91.59	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.17		Cheméo Relay (1.0)
logp	3.121		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	1914.00		NIST Webbook
tb	600.07	K	Cheméo Relay (1.0)
tf	275.81	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320838&Units=SI

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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