D-Proline, N-ethoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C10H17NO4/c1-3-14-9(12)8-6-5-7-11(8)10(13)15-4-2/h8H,3-7H2,1-2H3
InchiKey: GQDLZFPIOGXLCK-UHFFFAOYSA-N
Formula: C10H17NO4
SMILES: CCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 215.25

Physical Properties

Property code	Value	Unit	Source
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-1.14		Cheméo Relay (1.0)
logp	1.170		Crippen Method
mcvol	165.760	ml/mol	McGowan Method
rinpol	1516.00		NIST Webbook
rinpol	1516.00		NIST Webbook
tb	555.87	K	Cheméo Relay (1.0)
tf	286.18	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=U320834&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
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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