d-Proline, N-methoxycarbonyl-, methyl ester

Inchi: InChI=1S/C8H13NO4/c1-12-7(10)6-4-3-5-9(6)8(11)13-2/h6H,3-5H2,1-2H3
InchiKey: SRFMYIWPQPIVPO-UHFFFAOYSA-N
Formula: C8H13NO4
SMILES: COC(=O)C1CCCN1C(=O)OC
Mol. weight [g/mol]: 187.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.45		Crippen Method
logp	0.390		Crippen Method
mcvol	137.580	ml/mol	McGowan Method
rinpol	1433.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320785&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices