L-Proline, N-(5-chlorovaleryl)-, methyl ester

Inchi: InChI=1S/C11H18ClNO3/c1-16-11(15)9-5-4-8-13(9)10(14)6-2-3-7-12/h9H,2-8H2,1H3
InchiKey: OBAXQHFPWSIRJV-UHFFFAOYSA-N
Formula: C11H18ClNO3
SMILES: COC(=O)C1CCCN1C(=O)CCCCCl
Mol. weight [g/mol]: 247.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Cheméo Relay (1.0)
logp	1.560		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tf	328.96	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=U299717&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point