

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

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