L-Proline, N-pivaloyl-, methyl ester

Inchi: InChI=1S/C11H19NO3/c1-11(2,3)10(14)12-7-5-6-8(12)9(13)15-4/h8H,5-7H2,1-4H3
InchiKey: IXKVOAVZVBVJHK-UHFFFAOYSA-N
Formula: C11H19NO3
SMILES: COC(=O)C1CCCN1C(=O)C(C)(C)C
Mol. weight [g/mol]: 213.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.13		Cheméo Relay (1.0)
logp	1.196		Crippen Method
mcvol	173.980	ml/mol	McGowan Method
rinpol	1510.00		NIST Webbook
tf	316.72	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299745&Units=SI
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

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