1-(1-Methoxycarbonyl-2-methylpropyl)-2-isopropo

Inchi: InChI=1S/C9H18N2O4/c1-6(2)8(9(12)14-5)11(13)10-15-7(3)4/h6-8H,1-5H3/b11-10-
InchiKey: XSZJBNBXQSOURW-KHPPLWFESA-N
Formula: C9H18N2O4
SMILES: COC(=O)C(C(C)C)[N+]([O-])=NOC(C)C
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	1.486		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
rinpol	1409.00		NIST Webbook
rinpol	1409.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R121341&Units=SI
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.