1-(1-Isopropoxycarbonyl-2-methylpropyl)-2-isopro

Inchi: InChI=1S/C11H22N2O4/c1-7(2)10(11(14)16-8(3)4)13(15)12-17-9(5)6/h7-10H,1-6H3/b13
InchiKey: BSHZYTXHTGDYLF-SEYXRHQNSA-N
Formula: C11H22N2O4
SMILES: CC(C)ON=[N+]([O-])C(C(=O)OC(C)C)C(C)C
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	2.265		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R121287&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.