1-(1-Methoxycarbonyl-1-ethylpropyl)-2-methoxydi

Inchi: InChI=1S/C8H16N2O4/c1-5-8(6-2,7(11)13-3)10(12)9-14-4/h5-6H2,1-4H3/b10-9-
InchiKey: ROYCLGATJAMTBH-KTKRTIGZSA-N
Formula: C8H16N2O4
SMILES: CCC(CC)(C(=O)OC)[N+]([O-])=NOC
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	1.242		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
rinpol	1378.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R121301&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices