1-(1-Methoxycarbonyl-1-methylpropyl)-2-methoxy

Inchi: InChI=1S/C7H14N2O4/c1-5-7(2,6(10)12-3)9(11)8-13-4/h5H2,1-4H3/b9-8-
InchiKey: JPIAQTFJDLGBTA-HJWRWDBZSA-N
Formula: C7H14N2O4
SMILES: CCC(C)(C(=O)OC)[N+]([O-])=NOC
Mol. weight [g/mol]: 190.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.95		Crippen Method
logp	0.852		Crippen Method
mcvol	144.330	ml/mol	McGowan Method
rinpol	1304.00		NIST Webbook

Sources

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=R121336&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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