1-(1-Methoxycarbonyl-1-methylethyl)-2-methoxyd

Inchi: InChI=1S/C6H12N2O4/c1-6(2,5(9)11-3)8(10)7-12-4/h1-4H3/b8-7-
InchiKey: DQIYPXKYMGJNMT-FPLPWBNLSA-N
Formula: C6H12N2O4
SMILES: CON=[N+]([O-])C(C)(C)C(=O)OC
Mol. weight [g/mol]: 176.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.54		Crippen Method
logp	0.462		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
rinpol	1216.00		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=R121321&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