1-(1-Methoxycarbonyl-1-methylethyl)-2-butoxydia

Inchi: InChI=1S/C9H18N2O4/c1-5-6-7-15-10-11(13)9(2,3)8(12)14-4/h5-7H2,1-4H3/b11-10-
InchiKey: IAZQFCUNNXOIBG-KHPPLWFESA-N
Formula: C9H18N2O4
SMILES: CCCCON=[N+]([O-])C(C)(C)C(=O)OC
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	1.632		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
rinpol	1448.00		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=R121316&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