1-Methoxycarbonyl(cyclohexyl)methyl-2-methoxy

Inchi: InChI=1S/C10H18N2O4/c1-15-9(13)10(6-4-3-5-7-10)8-12(14)11-16-2/h3-8H2,1-2H3/b12
InchiKey: OOEALTUKYGLMCQ-QXMHVHEDSA-N
Formula: C10H18N2O4
SMILES: CON=[N+]([O-])CC1(C(=O)OC)CCCCC1
Mol. weight [g/mol]: 230.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.634		Crippen Method
mcvol	175.740	ml/mol	McGowan Method
rinpol	1682.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R390255&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

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