1-(1-Methoxycarbonylcyclohexyl)-2-methoxydiaze

Inchi: InChI=1S/C9H16N2O4/c1-14-8(12)9(11(13)10-15-2)6-4-3-5-7-9/h3-7H2,1-2H3/b11-10-
InchiKey: QXGLTTMKARCCPZ-KHPPLWFESA-N
Formula: C9H16N2O4
SMILES: CON=[N+]([O-])C1(C(=O)OC)CCCCC1
Mol. weight [g/mol]: 216.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	1.386		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
rinpol	1565.00		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=R121376&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