1-(1-Isopropoxycarbonylethyl)-2-isopropoxydiaze

Inchi: InChI=1S/C9H18N2O4/c1-6(2)14-9(12)8(5)11(13)10-15-7(3)4/h6-8H,1-5H3
InchiKey: JEWCOMLIOHMONS-UHFFFAOYSA-N
Formula: C9H18N2O4
SMILES: CC(C)ON=[N+]([O-])C(C)C(=O)OC(C)C
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.629		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
rinpol	1378.00		NIST Webbook
rinpol	1378.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R121292&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.