1-(2-Ethoxycarbonylethyl)-2-methoxydiazen-1-oxi

Inchi: InChI=1S/C6H12N2O4/c1-3-12-6(9)4-5-8(10)7-11-2/h3-5H2,1-2H3
InchiKey: XABIZHLHKBMYHC-UHFFFAOYSA-N
Formula: C6H12N2O4
SMILES: CCOC(=O)CC[N+]([O-])=NOC
Mol. weight [g/mol]: 176.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	0.463		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
rinpol	1246.00		NIST Webbook
rinpol	1246.00		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=R121445&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

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