

1-(1-Ethoxycarbonylpropyl)-2-ethoxydiazene-1-oxide

Inchi: InChI=1S/C8H16N2O4/c1-4-7(8(11)13-5-2)10(12)9-14-6-3/h7H,4-6H2,1-3H3/b10-9-
InchiKey: APUNMGYFYASDKN-KTKRTIGZSA-N
Formula: C8H16N2O4
SMILES: CCON=[N+](O-)C(CC)C(=O)OCC
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	1.242		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
rinpol	1382.00		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=R121267&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

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