

1-(1-Ethoxycarbonylethyl)-2-ethoxydiazene-1-oxide

Inchi: InChI=1S/C7H14N2O4/c1-4-12-7(10)6(3)9(11)8-13-5-2/h6H,4-5H2,1-3H3/b9-8-
InchiKey: GSPWRZWDFXPGRM-HJWRWDBZSA-N
Formula: C7H14N2O4
SMILES: CCON=[N+](O-)C(C)C(=O)OCC
Mol. weight [g/mol]: 190.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.95		Crippen Method
logp	0.852		Crippen Method
mcvol	144.330	ml/mol	McGowan Method
rinpol	1318.00		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=R121252&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

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