

1-Ethoxycarbonylmethyl-2-ethoxydiazene-1-oxide

Inchi: InChI=1S/C6H12N2O4/c1-3-11-6(9)5-8(10)7-12-4-2/h3-5H2,1-2H3
InchiKey: KHPPOLRTXIPFHE-UHFFFAOYSA-N
Formula: C6H12N2O4
SMILES: CCON=[N+](O-)CC(=O)OCC
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	1313.00		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=R121485&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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