

1-Methoxycarbonylmethyl-2-ethoxydiazene-1-oxide

Inchi: InChI=1S/C5H10N2O4/c1-3-11-6-7(9)4-5(8)10-2/h3-4H2,1-2H3/b7-6-
InchiKey: DTVQGSANPRCHOD-SREVYHEPSA-N
Formula: C5H10N2O4
SMILES: CCON=[N+](O-)[C@@H](C(=O)OC
Mol. weight [g/mol]: 162.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69e-03		Crippen Method
logp	0.073		Crippen Method
mcvol	116.150	ml/mol	McGowan Method
rinpol	1263.00		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=R121514&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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<https://www.chemeo.com/cid/69-416-4/1-Methoxycarbonylmethyl-2-ethoxydiazene-1-oxide.pdf>

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