

1-Methoxycarbonylmethyl-2-methoxydiazene-1-oxide

Inchi:	InChI=1S/C4H8N2O4/c1-9-4(7)3-6(8)5-10-2/h3H2,1-2H3
InchiKey:	XLRYDCNJOHAIED-UHFFFAOYSA-N
Formula:	C4H8N2O4
SMILES:	CON=[N+](O-)CC(=O)OC
Mol. weight [g/mol]:	148.12

Physical Properties

Property code	Value	Unit	Source
log10ws	0.41		Crippen Method
logp	-0.317		Crippen Method
mcvol	102.060	ml/mol	McGowan Method
rinsol	1184.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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<https://www.chemeo.com/cid/52-393-8/1-Methoxycarbonylmethyl-2-methoxydiazene-1-oxide.pdf>

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