

1-(1-Methoxycarbonylethyl)-2-isopropoxydiazene-1

Inchi: InChI=1S/C7H14N2O4/c1-5(2)13-8-9(11)6(3)7(10)12-4/h5-6H,1-4H3
InchiKey: YXIGZFWFSAIPR-UHFFFAOYSA-N
Formula: C7H14N2O4
SMILES: COC(=O)C(C)[N+][O-]=NOC(C)C
Mol. weight [g/mol]: 190.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	0.850		Crippen Method
mcvol	144.330	ml/mol	McGowan Method
rinpol	1300.00		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=R121405&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

Latest version available from:

<https://www.chemeo.com/cid/18-651-9/1-1-Methoxycarbonylethyl-2-isopropoxydiazene-1-oxide.pdf>

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