

1-(1-Methoxycarbonyl-1-methylethyl)-2-butoxydia

Inchi:	InChI=1S/C9H18N2O4/c1-5-6-7-15-10-11(13)9(2,3)8(12)14-4/h5-7H2,1-4H3/b11-10-
InchiKey:	IAZQFCUNNXOIBG-KHPPLWFESA-N
Formula:	C9H18N2O4
SMILES:	CCCCON=[N+](O-)C(C)(C)C(=O)OC
Mol. weight [g/mol]:	218.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	1.632		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
rinpol	1448.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R121316&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/44-379-3/1-1-Methoxycarbonyl-1-methylethyl-2-butoxydiazene-1-oxide.pdf>

Generated by Cheméo on 2024-04-20 12:18:37.353046669 +0000 UTC m=+15904766.273623982.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.