

Oxaziridine, 2-methyl-3-propyl-

Inchi:	InChI=1S/C5H11NO/c1-3-4-5-6(2)7-5/h5H,3-4H2,1-2H3
InchiKey:	QDNVKESMWRZQC-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CCCC1ON1C
Mol. weight [g/mol]:	101.15
CAS:	58751-77-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	0.990		Crippen Method
mcvol	86.300	ml/mol	McGowan Method

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=C58751772&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/82-404-2/Oxaziridine-2-methyl-3-propyl.pdf>

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