

4-Methylhydrazonomethyl-2,2,5,5-tetramethyl-3-imidazoline-1-oxyl

Inchi:	InChI=1S/C9H17N4O/c1-8(2)7(6-11-10-5)12-9(3,4)13(8)14/h6,10H,1-5H3
InchiKey:	OAFHDANZTSSHNS-UHFFFAOYSA-N
Formula:	C9H17N4O
SMILES:	CNN=CC1=NC(C)(C)N([O])C1(C)C
Mol. weight [g/mol]:	197.26
CAS:	64180-45-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.16		Crippen Method
logp	0.808		Crippen Method
mcvol	161.850	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=C64180456&Units=SI

Legend

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

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