

3-Carboxy-2,2,5,5-tetramethyl-1-pyrrolidinyloxy

Other names:	3-Carboxy-proxyl, free radical 2,2,5,5-Tetramethyl-1-pyrrolidinyl-oxy-3-carboxylic acid 3-Carboxy-proxyl 1-Pyrrolidinyloxy, 3-carboxy-2,2,5,5-tetramethyl- 2,2,5,5-Tetramethyl-3-carboxypyrrolidine-N-oxyl 2,2,5,5-Tetramethyl-3-carboxypyrrolidinoxy 3-Carboxy-2,2,5,5-tetramethylpyrrolidinyloxyl PCA 2,2,5,5-Tetramethylpiperidine-1-oxyl-3-carboxylic acid 2,2,5,5-Tetramethylpyrrolidine-1-oxyl-3-carboxylic acid 3-Carboxy-2,2,5,5-tetramethylpyrrolidin-1-oxy 3-Carboxy-2,2,5,5-tetramethylpyrrolidine-1-oxyl NSC 158842 PCA (radical) T 517 3-carboxy-2,2,5,5-tetramethylpyrrolidin-1-yloxy
Inchi:	InChI=1S/C9H16NO3/c1-8(2)5-6(7(11)12)9(3,4)10(8)13/h6H,5H2,1-4H3,(H,11,12)
InchiKey:	GEPIUTWNBHBHIO-UHFFFAOYSA-N
Formula:	C9H16NO3
SMILES:	CC1(C)CC(C(=O)O)C(C)(C)N1[O]
Mol. weight [g/mol]:	186.23
CAS:	2154-68-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.02		Crippen Method
logp	1.296		Crippen Method
mcvol	147.950	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

Legend

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

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