

1H-Pyrrol-1-yloxy, 3-(aminocarbonyl)-2,5-dihydro-2,2,5,5-tetramethyl-

Other names:	3-Pyrrolin-1-yloxy, 3-carbamoyl-2,2,5,5-tetramethyl- 2,2,5,5-Tetramethyl-3-carbamidopyrroline 1-oxyl 2,2,5,5-Tetramethyl-3-pyrrolin-1-yloxy-3-carboxamide 3-Carbamoyl-2,2,5,5-tetramethylpyrrolinoxyl 3-carbamoyl-2,2,5,5-tetramethyl-1H-pyrrol-1-yloxy
Inchi:	InChI=1S/C9H15N2O2/c1-8(2)5-6(7(10)12)9(3,4)11(8)13/h5H,1-4H3,(H2,10,12)
InchiKey:	RUEXQFPLRRIFTI-UHFFFAOYSA-N
Formula:	C9H15N2O2
SMILES:	CC1(C)C=C(C(N)=O)C(C)(C)N1[O]
Mol. weight [g/mol]:	183.23
CAS:	3229-73-0

Physical Properties

Property code	Value	Unit	Source
ie	7.40 ± 0.05	eV	NIST Webbook
log10ws	-6.22		Crippen Method
logp	0.616		Crippen Method
mcvol	147.760	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3229730&Units=SI
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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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