1-Pyrrolidinyloxy, 3-(aminocarbonyl)-2,2,5,5-tetramethyl-

Other names: 1-Pyrrolidinyloxy, 3-carbamoyl-2,2,5,5-tetramethyl-
2,2,5,5-Tetramethyl-3-carbamoyl-1-pyrrolidinyloxy
3-Carbamoyl-2,2,5,5-tetramethylpyrrolidine-1-oxyl
3-Carbamoyl-2,2,5,5-tetramethylpyrrolidinooxyl
3-carbamoyl-2,2,5,5-tetramethylpyrrolidin-1-yloxy

Inchi: InChI=1S/C9H17N2O2/c1-8(2)5-6(7(10)12)9(3,4)11(8)13/h6H,5H2,1-4H3,(H2,10,12)

InchiKey: XNNPAWRINYCIHL-UHFFFAOYSA-N

Formula: C9H17N2O2

SMILES: CC1(C)CC(C(N)=O)C(C)(C)N1[O]

Mol. weight [g/mol]: 185.24

CAS: 4399-80-8

Physical Properties

Property code	Value	Unit	Source
ie	7.40 ± 0.05	eV	NIST Webbook
log10ws	-6.13		Crippen Method
logp	0.696		Crippen Method
mcvol	152.060	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C4399808&Units=SI

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume