N-tert-Butoxycarbonyl-4-piperidone

Other names:	1-Piperidinecarboxylic acid, 4-oxo-, 1,1-dimethylethyl ester
Inchi:	InChI=1S/C10H17NO3/c1-10(2,3)14-9(13)11-6-4-8(12)5-7-11/h4-7H2,1-3H3
InchiKey:	ROUYFJUVMYHXFJ-UHFFFAOYSA-N
Formula:	C10H17NO3
SMILES:	CC(C)(C)OC(=O)N1CCC(=O)CC1
Mol. weight [g/mol]:	199.25
CAS:	79099-07-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	1.586		Crippen Method
mcvol	159.890	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=C79099073&Units=SI

Legend

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