

Pyrrolidine, 1-(2,2,4-trimethyl-3-oxovaleryl)-

Inchi:	InChI=1S/C12H21NO2/c1-9(2)10(14)12(3,4)11(15)13-7-5-6-8-13/h9H,5-8H2,1-4H3
InchiKey:	QCMUKRBNJZARHX-UHFFFAOYSA-N
Formula:	C12H21NO2
SMILES:	CC(C)C(=O)C(C)(C)C(=O)N1CCCC1
Mol. weight [g/mol]:	211.30
CAS:	91690-82-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.860		Crippen Method
mcvol	182.200	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91690823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/93-702-9/Pyrrolidine-1-2-2-4-trimethyl-3-oxovaleryl.pdf>

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