

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

Inchi:	InChI=1S/C13H23NO2/c1-10(2)11(15)13(3,4)12(16)14-8-6-5-7-9-14/h10H,5-9H2,1-4H3
InchiKey:	SLTCQIMTEMTYEH-UHFFFAOYSA-N
Formula:	C13H23NO2
SMILES:	CC(C)C(=O)C(C)(C)C(=O)N1CCCCC1
Mol. weight [g/mol]:	225.33
CAS:	73790-84-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	2.250		Crippen Method
mcvol	196.290	ml/mol	McGowan Method

Sources

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=C73790848&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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