

# 1-(2,4,6-Trinitrophenyl)piperidine

<b>Other names:</b>	N-(2,4,6-trinitrophenyl)piperidine
<b>Inchi:</b>	InChI=1S/C11H12N4O6/c16-13(17)8-6-9(14(18)19)11(10(7-8)15(20)21)12-4-2-1-3-5-12/
<b>InchiKey:</b>	PELVDFPFGQPDGS-UHFFFAOYSA-N
<b>Formula:</b>	C11H12N4O6
<b>SMILES:</b>	O=[N+]([O-])c1cc([N+](=O)[O-])c(N2CCCCC2)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	296.24
<b>CAS:</b>	67263-27-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	2.401		Crippen Method
mcvol	193.470	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C67263278&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C67263278&amp;Units=SI</a>

## Legend

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

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