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

Other names: N-(2,4,6-trinitrophenyl)piperidine
Inchi: 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/
InchiKey: PELVDFPFGQPDGS-UHFFFAOYSA-N
Formula: C11H12N4O6
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(N2CCCCC2)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 296.24
CAS: 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

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=C67263278&Units=SI

Legend

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