Piperidine, 1-(2,4-dinitrophenyl)-

Other names: 1-(2,4-dinitrophenyl)piperidine
Inchi: InChI=1S/C11H13N3O4/c15-13(16)9-4-5-10(11(8-9)14(17)18)12-6-2-1-3-7-12/h4-5,8H,1-
InchiKey: MPGYUYKSTWTQFS-UHFFFAOYSA-N
Formula: C11H13N3O4
SMILES: O=[N+]([O-])c1ccc(N2CCCCC2)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 251.24
CAS: 839-93-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	2.493		Crippen Method
mcvol	176.050	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=C839930&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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