

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

Inchi:	InChI=1S/C14H19N3O4/c1-2-3-11-6-8-15(9-7-11)13-5-4-12(16(18)19)10-14(13)17(20)21
InchiKey:	LPHVJKBVQMLKDM-UHFFFAOYSA-N
Formula:	C14H19N3O4
SMILES:	CCCC1CCN(c2ccc([N+](=O)[O-])cc2[N+](=O)[O-])CC1
Mol. weight [g/mol]:	293.32
CAS:	19780-01-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	3.519		Crippen Method
mcvol	218.320	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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<https://www.chemeo.com/cid/120-854-0/Piperidine-1-2-4-dinitrophenyl-4-propyl.pdf>

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