

Adenine, n-(p-nitrophenyl)-

Inchi:	InChI=1S/C11H8N6O2/c18-17(19)8-3-1-7(2-4-8)16-11-9-10(13-5-12-9)14-6-15-11/h1-6H
InchiKey:	GKYHZIPVNFXXJO-UHFFFAOYSA-N
Formula:	C11H8N6O2
SMILES:	O=[N+]([O-])c1ccc(Nc2ncnc3[nH]cnc23)cc1
Mol. weight [g/mol]:	256.22
CAS:	136112-69-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	1.523		Crippen Method
mcvol	170.490	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=C136112691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/74-436-6/Adenine-n-p-nitrophenyl.pdf>

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