

1H-Tetrazole, 1-(4-nitrophenyl)-

Other names:	1-(4-Nitrophenyl)-1h-tetrazole
Inchi:	InChI=1S/C7H5N5O2/c13-12(14)7-3-1-6(2-4-7)11-5-8-9-10-11/h1-5H
InchiKey:	NHYHTYJIILODSA-UHFFFAOYSA-N
Formula:	C7H5N5O2
SMILES:	O=[N+]([O-])c1ccc(-n2cnnn2)cc1
Mol. weight [g/mol]:	191.15
CAS:	14213-11-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	0.570		Crippen Method
mcvol	123.610	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=C14213117&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

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<https://www.chemeo.com/cid/38-333-0/1H-Tetrazole-1-4-nitrophenyl.pdf>

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