1H-1,2,4-triazole, 3-nitro-

Other names:	s-Triazole, 3-nitro-
	3-Nitro-1,2,4-triazole
	3-Nitro-1H-1,2,4-triazole
	3-Nitro-4H-[1,2,4]triazole
Inchi:	InChI=1S/C2H2N4O2/c7-6(8)2-3-1-4-5-2/h1H,(H,3,4,5)
InchiKey:	KUEFXPHXHHANKS-UHFFFAOYSA-N
Formula:	C2H2N4O2
SMILES:	O=[N+]([O-])c1nc[nH]n1
Mol. weight [g/mol]:	114.06

Physical Properties

Property code	Value	Unit	Source
logp	-0.769		Crippen Method
mcvol	66.940	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24807554&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume