

1H-Benzotriazole, 5-nitro-

Other names:	5-Nitrobenzo-1,2,3-triazole 5-Nitrobenzotriazole 1H-Benzotriazole, 6-nitro- 5-Nitro-1H-benzotriazole 5-Nitrobenzotriazol UN 0385 5-Nitro-1H-1,2,3-benzotriazole 6-Nitro-1H-benzotriazole NSC 3132 NSC 66476
Inchi:	InChI=1S/C6H4N4O2/c11-10(12)4-1-2-5-6(3-4)8-9-7-5/h1-3H,(H,7,8,9)
InchiKey:	AOCDQWRMYHJTMU-UHFFFAOYSA-N
Formula:	C6H4N4O2
SMILES:	O=[N+](O-)[c1ccc2[nH]nnc2c1]
Mol. weight [g/mol]:	164.12
CAS:	2338-12-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	0.384		Crippen Method
mcpol	103.840	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2338127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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