

6-Chloro-4-nitro-benzo-1,2,3-triazole

Other names:	6-chloro-4-nitro-1H-benzotriazole
Inchi:	InChI=1S/C6H3ClN4O2/c7-3-1-4-6(9-10-8-4)5(2-3)11(12)13/h1-2H,(H,8,9,10)
InchiKey:	HRBBUEDJKCLTQE-UHFFFAOYSA-N
Formula:	C6H3ClN4O2
SMILES:	O=[N+]([O-])c1cc(Cl)cc2[nH]nnc12
Mol. weight [g/mol]:	198.57
CAS:	13091-80-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	1.038		Crippen Method
mcvol	116.080	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=C13091800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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