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/ci990307l

Legend

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