1H-Indazole, 6-nitro-

Other names:	6-Nitroindazole
	6-Nitro-1H-indazole
	6-Nitroisoindazole
Inchi:	InChI=1S/C7H5N3O2/c11-10(12)6-2-1-5-4-8-9-7(5)3-6/h1-4H,(H,8,9)
InchiKey:	ORZRMRUXSPNQQL-UHFFFAOYSA-N
Formula:	C7H5N3O2
SMILES:	O=[N+]([O-])c1ccc2cn[nH]c2c1
Mol. weight [g/mol]:	163.13
CAS:	7597-18-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	0.989		Crippen Method
mcvol	107.950	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7597184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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