2-Methyl-5-nitro-2H-indazole

Other names:	2H-Indazole, 2-methyl-5-nitro- 2H-Benzopyrazole, 2-methyl-5-nitro-
Inchi:	InChI=1S/C8H7N3O2/c1-10-5-6-4-7(11(12)13)2-3-8(6)9-10/h2-5H,1H3
InchiKey:	IWPBWVZEOVCZRX-UHFFFAOYSA-N
Formula:	C8H7N3O2
SMILES:	Cn1cc2cc([N+](=O)[O-])ccc2n1
Mol. weight [g/mol]:	177.16
CAS:	5228-48-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Crippen Method
logp	1.481		Crippen Method
mcvol	122.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5228488&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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