

Dibenzofuran, 3-nitro-

Other names:	3-Nitrodibenzofuran
Inchi:	InChI=1S/C12H7NO3/c14-13(15)8-5-6-10-9-3-1-2-4-11(9)16-12(10)7-8/h1-7H
InchiKey:	UVFAHDAUVZRVCC-UHFFFAOYSA-N
Formula:	C12H7NO3
SMILES:	O=[N+](O-)c1ccc2c(c1)oc1cccc12
Mol. weight [g/mol]:	213.19
CAS:	5410-97-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.46		Crippen Method
logp	3.494		Crippen Method
mcvol	144.850	ml/mol	McGowan Method
rinpol	333.92		NIST Webbook
rinpol	333.80		NIST Webbook
rinpol	336.00		NIST Webbook
rinpol	336.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5410979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices

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