

Benzofurazan, 4-nitro-

Other names:	4-Nitrobenzofurazan
Inchi:	InChI=1S/C6H3N3O3/c10-9(11)5-3-1-2-4-6(5)8-12-7-4/h1-3H
InchiKey:	ZCVAGTPWBAXAL-UHFFFAOYSA-N
Formula:	C6H3N3O3
SMILES:	O=[N+](O-)c1cccc2nonc12
Mol. weight [g/mol]:	165.11
CAS:	16322-19-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.19		Crippen Method
logp	1.131		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16322193&Units=SI

Legend

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

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<https://www.chemeo.com/cid/112-631-6/Benzofurazan-4-nitro.pdf>

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