

Benzofurazan

Other names:	Benzo-2,1,3-oxadiazole 2-Oxa-1,3-diaza-2H-isoindene 2,1,3-Benzoxadiazole 3,5-Cyclohexadiene-1,2-dione, dioxime, furazan 2,1,3-Benzoxadiazol
Inchi:	InChI=1S/C6H4N2O/c1-2-4-6-5(3-1)7-9-8-6/h1-4H
InchiKey:	AWBOSXFRPFZLOP-UHFFFAOYSA-N
Formula:	C6H4N2O
SMILES:	c1ccc2nonc2c1
Mol. weight [g/mol]:	120.11
CAS:	273-09-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.54		Crippen Method
logp	1.223		Crippen Method
mcvol	82.310	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C273096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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