

5-Nitrobenzisoxazole

Inchi:	InChI=1S/C7H4N2O3/c10-9(11)6-1-2-7-5(3-6)4-8-12-7/h1-4H
InchiKey:	TWOYWCWKYDYTIP-UHFFFAOYSA-N
Formula:	C7H4N2O3
SMILES:	O=[N+]([O-])c1ccc2oncc2c1
Mol. weight [g/mol]:	164.12
CAS:	39835-28-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.43		Crippen Method
logp	1.736		Crippen Method
mcvol	103.840	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=C39835284&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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