

6-Nitro-2-phenylindolizine

Inchi:	InChI=1S/C14H10N2O2/c17-16(18)14-7-6-13-8-12(9-15(13)10-14)11-4-2-1-3-5-11/h1-10
InchiKey:	MAHPGNZUNZRRFK-UHFFFAOYSA-N
Formula:	C14H10N2O2
SMILES:	O=[N+]([O-])c1ccc2cc(-c3ccccc3)cn2c1
Mol. weight [g/mol]:	238.24
CAS:	60891-76-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	3.514		Crippen Method
mcvol	172.840	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=C60891761&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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