

3H-naphth[1,2-d]imidazole, 3-(p-nitroanilino)-2-(p-nitrophenyl)-

Inchi:	InChI=1S/C23H15N5O4/c29-27(30)18-10-5-16(6-11-18)23-24-22-20-4-2-1-3-15(20)7-14
InchiKey:	OQCLRORBVFEXCLH-UHFFFAOYSA-N
Formula:	C23H15N5O4
SMILES:	O=[N+]([O-])c1ccc(Nn2c(-c3ccc([N+](=O)[O-])cc3)nc3c4ccccc4ccc32)cc1
Mol. weight [g/mol]:	425.40
CAS:	116401-68-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.01		Crippen Method
logp	5.548		Crippen Method
mcvol	293.810	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=C116401684&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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