

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

Inchi:	InChI=1S/C23H15BrN4O2/c24-17-8-10-18(11-9-17)26-27-22-20-4-2-1-3-15(20)7-14-21(2
InchiKey:	HICLYCNLRUCEFS-UHFFFAOYSA-N
Formula:	C23H15BrN4O2
SMILES:	O=[N+]([O-])c1ccc(-c2nc3ccc4ccccc4c3n2Nc2ccc(Br)cc2)cc1
Mol. weight [g/mol]:	459.30
CAS:	14135-28-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.52		Crippen Method
logp	6.402		Crippen Method
mcvol	293.890	ml/mol	McGowan Method

Sources

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=C14135285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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