

3H-naphth[1,2-d]imidazole, 3-(p-anisidino)-2-(p-methoxyphenyl)-

Inchi:	InChI=1S/C25H21N3O2/c1-29-20-12-7-18(8-13-20)25-26-24-22-6-4-3-5-17(22)9-16-23(2
InchiKey:	OODZQZQIWMQAAX-UHFFFAOYSA-N
Formula:	C25H21N3O2
SMILES:	COc1ccc(Nn2c(-c3ccc(OC)cc3)nc3c4ccccc4ccc32)cc1
Mol. weight [g/mol]:	395.45
CAS:	13847-93-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.95		Crippen Method
logp	5.749		Crippen Method
mvol	298.890	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=C13847933&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
mvol:	McGowan's characteristic volume

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