

4-P-bromoanilino-6-methyl-1,3,3a,7-tetrazaindene

Inchi:	InChI=1S/C12H10BrN5/c1-8-6-11(18-12(16-8)14-7-15-18)17-10-4-2-9(13)3-5-10/h2-7,17
InchiKey:	VSCXKFCALANVFG-UHFFFAOYSA-N
Formula:	C12H10BrN5
SMILES:	<chem>Cc1cc(Nc2ccc(Br)cc2)n2ncnc2n1</chem>
Mol. weight [g/mol]:	304.14
CAS:	100123-38-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	2.939		Crippen Method
mcvol	184.660	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100123384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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