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: Cc1cc(Nc2ccc(Br)cc2)n2ncnc2n1
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