4-Anilino-6-methyl-1,3,3a,7-tetrazaindene

Inchi:	InChI=1S/C12H11N5/c1-9-7-11(16-10-5-3-2-4-6-10)17-12(15-9)13-8-14-17/h2-8,16H,1H3
InchiKey:	RLASLOLCTAMGCE-UHFFFAOYSA-N
Formula:	C12H11N5
SMILES:	Cc1cc(Nc2ccccc2)n2ncnc2n1
Mol. weight [g/mol]:	225.25
CAS:	92017-89-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	2.176		Crippen Method
mcvol	167.160	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92017895&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

Latest version available from:
https://www.chemeo.com/cid/94-133-0/4-Anilino-6-methyl-1-3-3a-7-tetrazaindene.pdf
Generated by Cheméo on 2024-10-12 03:53:29.841740004 +0000 UTC m=+3286072.478709252.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.