

N,n'-bis-(4-(6-methyl)1,3,3a,7-tetrazaindenyl)-ethyl

Inchi:	InChI=1S/C14H16N10/c1-9-5-11(23-13(21-9)17-7-19-23)15-3-4-16-12-6-10(2)22-14-18-8
InchiKey:	RTYJHJVSHFWKFJ-UHFFFAOYSA-N
Formula:	C14H16N10
SMILES:	Cc1cc(NCCNc2cc(C)nc3ncnn23)n2ncnc2n1
Mol. weight [g/mol]:	324.34
CAS:	100883-07-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	0.703		Crippen Method
mcvol	230.080	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=C100883076&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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