

5-P-anisyl-7-oxo-1,2,3a,4-tetrazaindene

Inchi:	InChI=1S/C12H10N4O2/c1-18-9-4-2-8(3-5-9)10-6-11(17)12-13-7-14-16(12)15-10/h2-7,15
InchiKey:	LFRWNTYPAGZIMB-UHFFFAOYSA-N
Formula:	C12H10N4O2
SMILES:	COc1ccc(-c2cc(=O)c3ncnn3[nH]2)cc1
Mol. weight [g/mol]:	242.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	0.611		Crippen Method
mcvol	168.920	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=B6002147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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