

Adenine, n-[p-(methylthio)phenyl]-

Inchi:	InChI=1S/C12H11N5S/c1-18-9-4-2-8(3-5-9)17-12-10-11(14-6-13-10)15-7-16-12/h2-7H,1
InchiKey:	RLIKBBNNCGQLQX-UHFFFAOYSA-N
Formula:	C12H11N5S
SMILES:	CSc1ccc(Nc2ncnc3[nH]cnc23)cc1
Mol. weight [g/mol]:	257.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	2.337		Crippen Method
mcvol	183.510	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=B6008707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/85-596-7/Adenine-n-p-methylthio-phenyl.pdf>

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