

2,5-Bis(anilino)-1,3,4-thiadiazole

Inchi:	InChI=1S/C14H12N4S/c1-3-7-11(8-4-1)15-13-17-18-14(19-13)16-12-9-5-2-6-10-12/h1-10
InchiKey:	IFBVXTYQCVAAYLA-UHFFFAOYSA-N
Formula:	C14H12N4S
SMILES:	<chem>c1ccc(N=c2[nH][nH]c(=Nc3ccccc3)s2)cc1</chem>
Mol. weight [g/mol]:	268.34
CAS:	1152-54-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	1.905		Crippen Method
mcvol	197.410	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1152541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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