

Phenyl thiolcarbamic acid, 5-anilino-1,3,4-thia-diazol-2-yl ester

Inchi:	InChI=1S/C15H12N4OS2/c20-14(17-12-9-5-2-6-10-12)22-15-19-18-13(21-15)16-11-7-3-
InchiKey:	ONAYJCUFOYMMQA-UHFFFAOYSA-N
Formula:	C15H12N4OS2
SMILES:	OC(=Nc1ccccc1)Sc1n[nH]c(=Nc2ccccc2)s1
Mol. weight [g/mol]:	328.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.560		Crippen Method
mcvol	229.420	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=B6002372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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