

S-triazolo[1,5-a]pyrimidin-7-ol-, 5-phenyl- (keto form)

Inchi:	InChI=1S/C11H8N4O/c16-10-6-9(8-4-2-1-3-5-8)14-11-12-7-13-15(10)11/h1-5,7H,6H2
InchiKey:	KZRZBVZFWOPBIB-UHFFFAOYSA-N
Formula:	C11H8N4O
SMILES:	O=C1CC(c2ccccc2)=Nc2ncnn21
Mol. weight [g/mol]:	212.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.443		Crippen Method
mcvol	148.960	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6010343&Units=SI

Legend

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

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