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/ci990307l
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=B6010343&Units=SI

Legend

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