

5,8-Dihydro-5,8-ethano-2-phenyl-3-(1-phenyl-5'-tet

Inchi:	InChI=1S/C25H20N4O2S/c30-22-19-16-11-13-17(14-12-16)20(19)23(31)24(21(22)15-7-3
InchiKey:	FOVGYLKUPFWGNK-UHFFFAOYSA-N
Formula:	C25H20N4O2S
SMILES:	Oc1c(Sc2nnnn2-c2ccccc2)c(-c2ccccc2)c(O)c2c1C1C=CC2CC1
Mol. weight [g/mol]:	440.52
CAS:	5831-23-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.55		Crippen Method
logp	5.423		Crippen Method
mcvol	314.360	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=C5831232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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