

Triazolo [4,5-d] pyrimidine, 3h-v-, 7-(octyloxy)-

Inchi:	InChI=1S/C12H19N5O/c1-2-3-4-5-6-7-8-18-12-10-11(13-9-14-12)16-17-15-10/h9H,2-8H2
InchiKey:	QKLSRUHMQRNYCB-UHFFFAOYSA-N
Formula:	C12H19N5O
SMILES:	CCCCCCCCOc1ncnc2[nH]nnc12
Mol. weight [g/mol]:	249.31
CAS:	94523-45-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	2.005		Crippen Method
mcvol	196.790	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94523452&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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