

7H-pyrrolo[2,3-d]pyrimidine, 4-chloro-7-cyclopentyl-

Inchi:	InChI=1S/C11H12ClN3/c12-10-9-5-6-15(8-3-1-2-4-8)11(9)14-7-13-10/h5-8H,1-4H2
InchiKey:	ZQHBEEYPDFIIPH-UHFFFAOYSA-N
Formula:	C11H12ClN3
SMILES:	Clc1ncnc2c1ccn2C1CCCC1
Mol. weight [g/mol]:	221.69
CAS:	212268-44-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	3.200		Crippen Method
mcvol	158.250	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C212268445&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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