

5-Chloro-1,10-phenanthroline

Other names:	1,10-Phenanthroline, 5-chloro-
Inchi:	InChI=1S/C12H7ClN2/c13-10-7-8-3-1-5-14-11(8)12-9(10)4-2-6-15-12/h1-7H
InchiKey:	XDUUQOQFSWSZSM-UHFFFAOYSA-N
Formula:	C12H7ClN2
SMILES:	Clc1cc2cccnc2c2ncccc12
Mol. weight [g/mol]:	214.65
CAS:	4199-89-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	3.436		Crippen Method
mcvol	149.460	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=C4199897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/52-845-6/5-Chloro-1-10-phenanthroline.pdf>

Generated by Cheméo on 2025-12-25 15:21:56.219452243 +0000 UTC m=+6424313.749492897.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.