

5-Cyano-2-picoline

Inchi:	InChI=1S/C7H6N2/c1-6-2-3-7(4-8)5-9-6/h2-3,5H,1H3
InchiKey:	PBLOYQAQGYUPCM-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	Cc1ccc(C#N)cn1
Mol. weight [g/mol]:	118.14
CAS:	3222-48-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	1.262		Crippen Method
mcvol	97.090	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=C3222488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:

<https://www.chemeo.com/cid/60-747-6/5-Cyano-2-picoline.pdf>

Generated by Cheméo on 2025-12-05 16:29:15.954586016 +0000 UTC m=+4700353.484626671.

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