2-Chloro-3-cyano-6-methylpyridine

Inchi: InChI=1S/C7H5ClN2/c1-5-2-3-6(4-9)7(8)10-5/h2-3H,1H3
InchiKey: YSBNBAYNISAUIT-UHFFFAOYSA-N
Formula: C7H5ClN2
SMILES: Cc1ccc(C#N)c(Cl)n1
Mol. weight [g/mol]: 152.58
CAS: 28900-10-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	1.915		Crippen Method
mcvol	109.330	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28900109&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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