2-Cyano-6-methyl pyridine

Other names: 6-methylpyridine-2-carbonitrile
Inchi: InChI=1S/C7H6N2/c1-6-3-2-4-7(5-8)9-6/h2-4H,1H3
InchiKey: CMADFEQMYFNYCF-UHFFFAOYSA-N
Formula: C7H6N2
SMILES: Cc1cccc(C#N)n1
Mol. weight [g/mol]: 118.14
CAS: 1620-75-3

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=C1620753&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