

2-chloro-4-methylpyridine

Inchi: InChI=1S/C6H6ClN/c1-5-2-3-8-6(7)4-5/h2-4H,1H3
InchiKey: MZVSTDHRRYQFGI-UHFFFAOYSA-N
Formula: C6H6ClN
SMILES: Cc1ccnc(Cl)c1
Mol. weight [g/mol]: 127.57
CAS: 3678-62-4

Physical Properties

Property code	Value	Unit	Source
affp	921.20	kJ/mol	NIST Webbook
basg	889.40	kJ/mol	NIST Webbook
log10ws	-2.40		Crippen Method
logp	2.043		Crippen Method
mcvol	93.860	ml/mol	McGowan Method

Sources

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=C3678624&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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