2,3,4-Trimethylpyridine

Other names: Pyridine, 2,3,4-trimethyl-
Inchi: InChI=1S/C8H11N/c1-6-4-5-9-8(3)7(6)2/h4-5H,1-3H3
InchiKey: HOPRXXXSABQWAV-UHFFFAOYSA-N
Formula: C8H11N
SMILES: Cc1ccnc(C)c1C
Mol. weight [g/mol]: 121.18
CAS: 2233-29-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.007		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
rinpol	1084.00		NIST Webbook
rinpol	1099.00		NIST Webbook
ripol	1541.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2233296&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices