

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:	<chem>Cc1ccnc(C)c1C</chem>
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

Latest version available from:

<https://www.cheméo.com/cid/69-134-7/2-3-4-Trimethylpyridine.pdf>

Generated by Cheméo on 2024-04-23 14:35:50.650684472 +0000 UTC m=+16172199.571261785.

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