2,4,5-Trimethylpyridine

Other names:	Pyridine, 2,4,5-trimethyl-
Inchi:	InChI=1S/C8H11N/c1-6-4-8(3)9-5-7(6)2/h4-5H,1-3H3
InchiKey:	MNDSSKADVGDFDF-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	Cc1cc(C)c(C)cn1
Mol. weight [g/mol]:	121.18
CAS:	1122-39-0

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	1066.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1053.90		NIST Webbook
rinpol	1071.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1507.00		NIST Webbook
tb	456.65 ± 5.00	K	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=C1122390&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
tb:	Normal Boiling Point Temperature

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