Pyridine, 4-ethyl-2-methyl-

Other names:	4-ethyl-2-methylpyridine
	5-ethyl-2-methylpyridine
	Pyridine, 2-methyl-4-ethyl
Inchi:	InChI=1S/C8H11N/c1-3-8-4-5-9-7(2)6-8/h4-6H,3H2,1-2H3
InchiKey:	KNCHDRLWPAKSII-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCc1ccnc(C)c1
Mol. weight [g/mol]:	121.18
CAS:	536-88-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.952		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
rinpol	1033.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1043.00		NIST Webbook
ripol	1440.00		NIST Webbook
tb	453.15 ± 2.00	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46565e+01
Coeff. B	-3.87777e+03
Coeff. C	-6.68480e+01
Temperature range (K), min.	336.72
Temperature range (K), max.	481.80

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C536889&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature