

Pyridine, 4-ethyl-2,6-dimethyl-

Other names:	2,6-Dimethyl-4-ethylpyridine 4-Ethyl-2,6-dimethylpyridine
Inchi:	InChI=1S/C9H13N/c1-4-9-5-7(2)10-8(3)6-9/h5-6H,4H2,1-3H3
InchiKey:	YFCLFEIWFHJNFU-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCc1cc(C)nc(C)c1
Mol. weight [g/mol]:	135.21
CAS:	36917-36-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.261		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpol	1067.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1079.10		NIST Webbook
rinpol	1079.10		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32020e+01
Coeff. B	-3.50105e+03
Coeff. C	-6.92110e+01
Temperature range (K), min.	340.31
Temperature range (K), max.	512.91

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=C36917369&Units=SI
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/ci990307I

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

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