

4-Butyl pyridine

Other names:	Pyridine, 4-butyl- Pyridine, 4-n-butyl
Inchi:	InChI=1S/C9H13N/c1-2-3-4-9-5-7-10-8-6-9/h5-8H,2-4H2,1H3
InchiKey:	LWMDPZVQAMQFOC-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCCCc1ccncc1
Mol. weight [g/mol]:	135.21
CAS:	5335-75-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	2.424		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
rinpol	1123.00		NIST Webbook
rinpol	1124.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	481.20	K	99.10	NIST Webbook
tbrp	371.20	K	2.70	NIST Webbook

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=C5335751&Units=SI
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
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure

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