

Pyridine, 2-(1-butylpentyl)-

Other names:	2-(5-Nonyl)pyridine 2-(1-n-Butylpentyl)pyridine 2-(1-Butylpentyl)pyridine
Inchi:	InChI=1S/C14H23N/c1-3-5-9-13(10-6-4-2)14-11-7-8-12-15-14/h7-8,11-13H,3-6,9-10H2,1
InchiKey:	YGCMUHWXPXEZCR-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCCCC(CCCC)c1ccccn1
Mol. weight [g/mol]:	205.34
CAS:	2961-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	4.546		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
rinqol	1451.80		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2961491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinqol:	Non-polar retention indices

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