

4-(1-Butylpentyl)pyridine

Other names:	4-(5-Nonyl)pyridine Pyridine, 4-(1-butylpentyl)- 4-(Butylpentyl)pyridine
Inchi:	InChI=1S/C14H23N/c1-3-5-7-13(8-6-4-2)14-9-11-15-12-10-14/h9-13H,3-8H2,1-2H3
InchiKey:	ATCGHKBXRIOBDX-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCCCC(CCCC)c1ccncc1
Mol. weight [g/mol]:	205.34
CAS:	2961-47-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	4.546		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
rinpol	1545.20		NIST Webbook
rinpol	1545.20		NIST Webbook
tb	539.20	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2961479&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

rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

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