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]: 205.35

Physical Properties

Property code	Value	Unit	Source
ie	9.28	eV	Cheméo Relay (1.0)
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
tf	253.03	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2961479&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point