Pyridine, 3-octyl

Inchi: InChI=1S/C13H21N/c1-2-3-4-5-6-7-9-13-10-8-11-14-12-13/h8,10-12H,2-7,9H2,1H3
InchiKey: VRSLSMSXIFJONL-UHFFFAOYSA-N
Formula: C13H21N
SMILES: CCCCCCCCc1cccnc1
Mol. weight [g/mol]: 191.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	3.985		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
ripol	2034.00		NIST Webbook
ripol	2034.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R70535&Units=SI

Legend

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