Pyridine, 3-heptyl

Inchi: InChI=1S/C12H19N/c1-2-3-4-5-6-8-12-9-7-10-13-11-12/h7,9-11H,2-6,8H2,1H3
InchiKey: YQXWJSLWMQLIAC-UHFFFAOYSA-N
Formula: C12H19N
SMILES: CCCCCCCc1cccnc1
Mol. weight [g/mol]: 177.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	3.595		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
rinpol	1455.00		NIST Webbook
ripol	1925.00		NIST Webbook
ripol	1925.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R70517&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol: Polar retention indices

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