

4-heptylpyridine

Inchi:	InChI=1S/C12H19N/c1-2-3-4-5-6-7-12-8-10-13-11-9-12/h8-11H,2-7H2,1H3
InchiKey:	JOSRHPJBIOMTCK-UHFFFAOYSA-N
Formula:	C12H19N
SMILES:	CCCCCCCc1ccncc1
Mol. weight [g/mol]:	177.29
CAS:	40089-90-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	3.595		Crippen Method
mcvol	166.160	ml/mol	McGowan Method

Sources

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=C40089905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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