

Pyridine, 3-hexyl

Inchi: InChI=1S/C11H17N/c1-2-3-4-5-7-11-8-6-9-12-10-11/h6,8-10H,2-5,7H2,1H3
InchiKey: LWEQIZSFZFUWIE-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CCCCCC1CCCN1
Mol. weight [g/mol]: 163.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	3.204		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
rinpol	1350.00		NIST Webbook
ripol	1813.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R70521&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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<https://www.chemeo.com/cid/79-788-1/Pyridine-3-hexyl.pdf>

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