

Pyridine, 2-hexyl-

Other names:	2-Hexylpyridine Pyridine, 2-(n-hexyl)- 2-C ₆ H ₁₃ (c-C ₅ H ₄ N)
Inchi:	InChI=1S/C ₁₁ H ₁₇ N/c1-2-3-4-5-8-11-9-6-7-10-12-11/h6-7,9-10H,2-5,8H2,1H3
InchiKey:	NZLJDTKLZIMONR-UHFFFAOYSA-N
Formula:	C ₁₁ H ₁₇ N
SMILES:	CCCCCCc1ccccn1
Mol. weight [g/mol]:	163.26
CAS:	1129-69-7

Physical Properties

Property code	Value	Unit	Source
affp	963.60	kJ/mol	NIST Webbook
basg	931.70	kJ/mol	NIST Webbook
log10ws	-3.71		Crippen Method
logp	3.204		Crippen Method
mcvol	152.070	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1129697&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

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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