

2-(i-C3H7)-pyridine

Inchi:	InChI=1S/C8H11N/c1-7(2)8-5-3-4-6-9-8/h3-7H,1-2H3
InchiKey:	PFYPDUUXDADWKC-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CC(C)c1ccccc1
Mol. weight [g/mol]:	121.18
CAS:	75981-47-4

Physical Properties

Property code	Value	Unit	Source
affp	956.40	kJ/mol	NIST Webbook
basg	924.60	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	2.205		Crippen Method
mcvol	109.800	ml/mol	McGowan Method

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=C75981474&Units=SI

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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<https://www.chemeo.com/cid/70-994-1/2-i-C3H7-pyridine.pdf>

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