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)c1ccccn1
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