4-Isopropylpyridine

Other names:	Pyridine, 4-(1-methylethyl)-
	4-(1-Methylethyl)pyridine
	4-(i-C3H7)-C5H4N
Inchi:	InChI=1S/C8H11N/c1-7(2)8-3-5-9-6-4-8/h3-7H,1-2H3
InchiKey:	FRGXNJWEDDQLFH-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CC(C)c1ccncc1
Mol. weight [g/mol]:	121.18
CAS:	696-30-0

Physical Properties

Property code	Value	Unit	Source
affp	955.70	kJ/mol	NIST Webbook
basg	923.80	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	2.205		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
rinpol	1054.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1054.00		NIST Webbook
tb	446.20	K	NIST Webbook
tf	218.25 ± 0.50	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C696300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point