2-Pyridinecarboxylic acid, 5-butyl-

Other names:	Picolinic acid, 5-butyl-
	Fusaric acid
	5-n-Butylpyridine-2-carboxylic acid
	5-Butylpicolinic acid
	5-Butyl-2-pyridinecarboxylic acid
	Fusarinic acid
	5-butylpyridine-3-carboxylic acid
Inchi:	InChI=1S/C10H13NO2/c1-2-3-4-8-5-6-9(10(12)13)11-7-8/h5-7H,2-4H2,1H3,(H,12,13)
InchiKey:	DGMPVYSXXIOGJY-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCCc1ccc(C(=O)O)nc1
Mol. weight [g/mol]:	179.22
CAS:	536-69-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	2.122		Crippen Method
mcvol	145.420	ml/mol	McGowan Method

Sources

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=C536696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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