

3-(4-Pyridyl)acrylic acid

Other names:	2-Propenoic acid, 3-(4-pyridinyl)- 4-Pyridineacrylic acid
Inchi:	InChI=1S/C8H7NO2/c10-8(11)2-1-7-3-5-9-6-4-7/h1-6H,(H,10,11)/b2-1+
InchiKey:	SSAYTINUCCRGDR-OWOJBTEDSA-N
Formula:	C8H7NO2
SMILES:	O=C(O)C=Cc1ccncc1
Mol. weight [g/mol]:	149.15
CAS:	5337-79-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	1.179		Crippen Method
mcvol	112.940	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5337791&Units=SI
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

Legend

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/69-273-3/3-4-Pyridyl-acrylic-acid.pdf>

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