Ethyl 3-pyridylacetate

Other names:	3-Pyridineacetic acid, ethyl ester
	Acetic acid, 2-(3-pyridyl)-, ethyl ester
	Ethyl 3-pyridineacetate
Inchi:	InChI=1S/C9H11NO2/c1-2-12-9(11)6-8-4-3-5-10-7-8/h3-5,7H,2,6H2,1H3
InchiKey:	RPWXYCRIAGBAGY-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCOC(=O)Cc1cccnc1
Mol. weight [g/mol]:	165.19
CAS:	39931-77-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Crippen Method
logp	1.187		Crippen Method
mcvol	131.330	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	0.05	NIST Webbook

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=C39931776&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
tbrp:	Boiling point at reduced pressure

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