2-Pyridylacetonitrile

Other names:	Pyridine-2-acetonitrile
	2-Pyridineacetonitrile
Inchi:	InChI=1S/C7H6N2/c8-5-4-7-3-1-2-6-9-7/h1-3,6H,4H2
InchiKey:	UKVQBONVSSLJBB-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	N#CCc1ccccn1
Mol. weight [g/mol]:	118.14
CAS:	2739-97-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.148		Crippen Method
mcvol	97.090	ml/mol	McGowan Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
ripol	2020.00		NIST Webbook

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=C2739971&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

ripol: Polar retention indices