

3-Pyridineacetonitrile

Other names:	3-Cyanomethylpyridine 3-Pyridylacetonitrile
Inchi:	InChI=1S/C7H6N2/c8-4-3-7-2-1-5-9-6-7/h1-2,5-6H,3H2
InchiKey:	OIPHWUPMXHQWLR-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	N#CCc1cccnc1
Mol. weight [g/mol]:	118.14
CAS:	6443-85-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.148		Crippen Method
mcpvol	97.090	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	0.10	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=C6443852&Units=SI

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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