

Pyridine-3,4-dicarbonitrile

Other names:	3,4-Pyridinedicarbonitrile
Inchi:	InChI=1S/C7H3N3/c8-3-6-1-2-10-5-7(6)4-9/h1-2,5H
InchiKey:	ALJUMASAQKRVRM-UHFFFAOYSA-N
Formula:	C7H3N3
SMILES:	N#Cc1ccncc1C#N
Mol. weight [g/mol]:	129.12
CAS:	1633-44-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	0.825		Crippen Method
mcvol	98.470	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1633449&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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