2,3,5,6-Pyridinetetracarbonitrile

Inchi: InChI=1S/C9HN5/c10-2-6-1-7(3-11)9(5-13)14-8(6)4-12/h1H
InchiKey: RRZLWIPIQKXHAS-UHFFFAOYSA-N
Formula: C9HN5
SMILES: N#Cc1cc(C#N)c(C#N)nc1C#N
Mol. weight [g/mol]: 179.14
CAS: 17638-20-9

Physical Properties

Property code	Value	Unit	Source
ea	2.17 ± 0.07	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	0.568		Crippen Method
mcvol	129.410	ml/mol	McGowan Method

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=C17638209&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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