2,3-Dicyano-5-phenylpyrazine

Other names: 2,3-Pyrazinedicarbonitrile,5-phenyl-
Inchi: InChI=1S/C12H6N4/c13-6-10-11(7-14)16-12(8-15-10)9-4-2-1-3-5-9/h1-5,8H
InchiKey: KSVMJUBGOLBDJX-UHFFFAOYSA-N
Formula: C12H6N4
SMILES: N#Cc1ncc(-c2ccccc2)nc1C#N
Mol. weight [g/mol]: 206.20
CAS: 52109-66-7

Physical Properties

Property code	Value	Unit	Source
ie	8.68	eV	NIST Webbook
log10ws	-4.31		Crippen Method
logp	1.887		Crippen Method
mcvol	155.140	ml/mol	McGowan Method

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=C52109667&Units=SI

Legend

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

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