2,3-DICYANO-5-METHYL-6-PHENYLPYRAZINE

Other names: 2,3-Pyrazinedicarbonitrile, 5-methyl-6-phenyl-
Inchi: InChI=1S/C13H8N4/c1-9-13(10-5-3-2-4-6-10)17-12(8-15)11(7-14)16-9/h2-6H,1H3
InchiKey: YKYXESCSPXPMKE-UHFFFAOYSA-N
Formula: C13H8N4
SMILES: Cc1nc(C#N)c(C#N)nc1-c1ccccc1
Mol. weight [g/mol]: 220.24

Physical Properties

Property code	Value	Unit	Source
ie	8.65	eV	NIST Webbook
logp	2.195		Crippen Method
mcvol	169.230	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52109678&Units=SI

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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