

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:	<chem>Cc1nc(C#N)c(C#N)nc1-c1ccccc1</chem>
Mol. weight [g/mol]:	220.23
CAS:	52109-67-8

Physical Properties

Property code	Value	Unit	Source
ie	8.65	eV	NIST Webbook
log10ws	-4.79		Crippen Method
logp	2.195		Crippen Method
mcvol	169.230	ml/mol	McGowan Method

Sources

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

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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