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]: 206.21

Physical Properties

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

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52109667&Units=SI
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

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.