1,3-Cyclopentadiene, 5-diazo-

Other names: 1,3-Cyclopentadiene,5-diazo-
Cyclopentadiene, 5-diazo-
Diazocyclopentadiene
Inchi: InChI=1S/C5H4N2/c6-7-5-3-1-2-4-5/h1-4H
InchiKey: UETCMNDFHMOYSP-UHFFFAOYSA-N
Formula: C5H4N2
SMILES: [N-]=[N+]=C1C=CC=C1
Mol. weight [g/mol]: 92.10

Physical Properties

Property code	Value	Unit	Source
ie	8.09 ± 0.01	eV	NIST Webbook
ie	8.33	eV	NIST Webbook
logp	0.783		Crippen Method
mcvol	73.210	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192274&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

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