

2,5-Cyclohexadien-1-one, 4-diazo-

Other names:	p-Benzoquinone diazide 1,4-Benzoquinone diazide 4-Diazo-2,5-cyclohexadien-1-one p-Diazoquinone Quinone diazide p-Quinone diazide
Inchi:	InChI=1S/C6H4N2O/c7-8-5-1-3-6(9)4-2-5/h1-4H
InchiKey:	WTQZSMDDRMKJRI-UHFFFAOYSA-N
Formula:	C6H4N2O
SMILES:	[N-]=[N+]=C1C=CC(=O)C=C1
Mol. weight [g/mol]:	120.11
CAS:	932-97-8

Physical Properties

Property code	Value	Unit	Source
ie	8.28 ± 0.05	eV	NIST Webbook
log10ws	-2.85		Crippen Method
logp	0.352		Crippen Method
mcvol	88.870	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=C932978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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