Ethanone,2-diazo-1-(4-methylphenyl)-

Other names: p-Methyl-2-diazoacetophenone
Inchi: InChI=1S/C9H8N2O/c1-7-2-4-8(5-3-7)9(12)6-11-10/h2-6H,1H3
InchiKey: XJXHQFDKVHPDHF-UHFFFAOYSA-N
Formula: C9H8N2O
SMILES: Cc1ccc(C(=O)C=[N+]=[N-])cc1
Mol. weight [g/mol]: 160.17
CAS: 17263-64-8

Physical Properties

Property code	Value	Unit	Source
ie	8.80 ± 0.05	eV	NIST Webbook
log10ws	-4.25		Crippen Method
logp	1.478		Crippen Method
mcvol	126.840	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=C17263648&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