Compound Information

Chemical Names: 2-(4'-Chlorophenyl)-1,4-benzoquinone

4′-Chlorophenyl-2,5-benzoquinone

1-(4'-Chlorophenyl)-benzo-2,5-quinone

2-(4'-Chlorophenyl)cyclohexa-2,5-diene-1,4-dione

Chemical formula: $C_{12}H_7ClO_2$

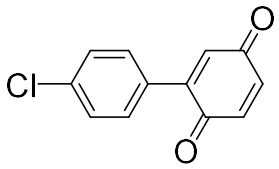
Molecular weight: 218.63

PubChem CID: 244141

InChl Key: ZYZNNQZZYJAPLH-UHFFFAOYSA-N

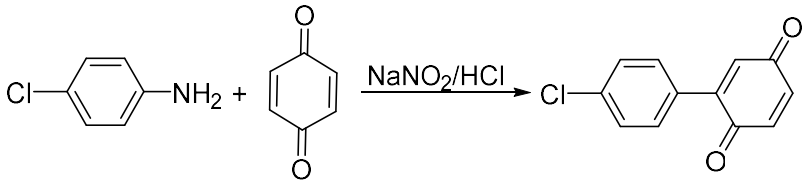
CAS number: 20307-43-1

Structure:



Synthesis: 2-(4-Chlorophenyl)-1,4-benzoquinone was synthesized from 1,4-benzoquinone and diazotized 4-chloroaniline using the Meerwein arylation as described previously (Amaro et al., 1996; Espandiari et al., 2004).

Reaction:



GC-MS: *m/z* 218.0, 183.1

Purity: > 99% by GC MS, detail of analysis method see reference (Li et al., 2018).

State: Yellow crystal

Instruments and software used to record and process raw data

Files	Instruments for raw data	Software to process raw data
GC-MS raw.D.rar	Mass spectra of all compounds were recorded on an Agilent 7890A gas chromatograph equipped with an Agilent 5975C Inert Mass Selective Detector (Agilent Technologies, CA, USA)	Agilent ChemStation is commonly used to process the raw data in .d format. Raw data can be converted into the desired format using ProteoWizard software.

Reference:

Amaro AR, Oakley GG, Bauer U, Spielmann HP & Robertson LW (1996) Metabolic activation of PCBs to quinones: Reactivity toward nitrogen and sulfur nucleophiles and influence of superoxide dismutase. Chem. Res. Toxicol. 9: 623-629

Espandiari P, Glauert HP, Lehmler HJ, Lee EY, Srinivasan C & Robertson LW (2004) Initiating activity of 4-chlorobiphenyl metabolites in the resistant hepatocyte model. Toxicol. Sci. 79: 41-46

Li X, Holland EB, Feng W, Zheng J, Dong Y, Pessah IN, Duffel MW, Robertson LW & Lehmler HJ (2018) Authentication of synthetic environmental contaminants and their (bio)transformation products in toxicology: polychlorinated biphenyls as an example. Environ Sci Pollut Res 25: 16508-16521