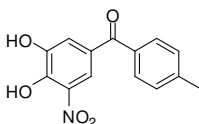




Certificate of Analysis

Axon Catalogue ID: 3993 **Batch Number:** 1
Product Name: Tolcapone
Alternative Name(s): Ro 40-7592
IUPAC Name: (3,4-Dihydroxy-5-nitrophenyl)(p-tolyl)methanone

Structure:



Amount:

CAS number(s): 134308-13-7
Molecular Formula: C₁₄H₁₁NO₅ **Molecular Weight:** 273.24
Batch Molecular Formula: C₁₄H₁₁NO₅·0.25H₂O **Batch Molecular Weight:** 277.74
Appearance: Yellow solid **Observed mp:** 145 °C
TLC (R_f): 0.39 DCM/MeOH (9:1)
Chemical Purity: 99.3%
¹H-NMR: Analytical data confirm chemical structure
Mass Spec: Analytical data confirm chemical structure
Microanalysis: Calculated: C 60.54, H 4.17, N 5.04; Found: C 60.89, H 4.06, N 5.05
Storage Conditions: Desiccate at -20 °C

| Solubility Data: | Solvent | Solubility (mg/ml) | Solubility (mM) | Remarks |
|-------------------------|----------------|---------------------------|------------------------|----------------|
| | Water | 0.0 | 0.0 | Insoluble |
| | 0.1N NaOH (aq) | | | Not Tested |
| | 0.1N HCl (aq) | | | Not Tested |
| | DMSO | 27.8 | >100 mM | |
| | EtOH | 27.8 | >100 mM | |

Remarks:

QC Date: 20-9-2023

The purity of Axon Ligands is confirmed by HPLC, MS, NMR and/or microanalysis. Analytical data are available upon request. Request can be submitted by e-mail to info@axonmedchem.com indicating Catalogue ID and Batch number.

Caution: Not fully tested. For research purposes only