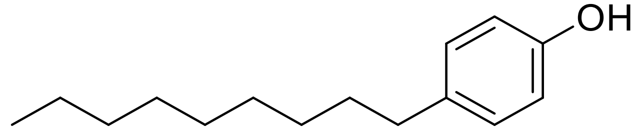
Product data sheet

MedKoo Cat#: 591913 Name: 4-n-Nonylphenol CAS#: 104-40-5 (4-n-Nonyl phenol) Chemical Formula: $C_{15}H_{24}O$ Exact Mass: 220.1827 Molecular Weight: 220.36		
Product supplied as:	Powder	
Purity (by HPLC):	≥ 98%	
Shipping conditions	Ambient temperature	
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.	

1. Product description:

Nonylphenols are a family of closely related organic compounds composed of phenol bearing a 9 carbon-tail. Nonylphenols can come in numerous structures, all of which may be considered alkylphenols. They are used in manufacturing antioxidants, lubricating oil additives, laundry and dish detergents, emulsifiers, and solubilizers. They are used extensively in epoxy formulation in North America but its use has been phased out in Europe. These compounds are also precursors to the commercially important non-ionic surfactants alkylphenol ethoxylates and nonylphenol ethoxylates, which are used in detergents, paints, pesticides, personal care products, and plastics. Nonylphenol has attracted attention due to its prevalence in the environment and its potential role as an endocrine disruptor and xenoestrogen, due to its ability to act with estrogen-like activity. The estrogenicity and biodegradation heavily depends on the branching of the nonyl sidechain. Nonylphenol has been found to act as an agonist of the GPER (GPR30).

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	TBD	TBD

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	4.54 mL	22.69 mL	45.38 mL
5 mM	0.91 mL	4.54 mL	9.08 mL
10 mM	0.45 mL	2.27 mL	4.54 mL
50 mM	0.09 mL	0.45 mL	0.91 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Bonefeld-Jørgensen EC, Long M, Hofmeister MV, Vinggaard AM. Endocrine-disrupting potential of bisphenol A, bisphenol A dimethacrylate, 4-n-nonylphenol, and 4-n-octylphenol in vitro: new data and a brief review. Environ Health Perspect. 2007 Dec;115 Suppl 1(Suppl 1):69-76. doi: 10.1289/ehp.9368. PMID: 18174953; PMCID: PMC2174402.
2. Ji X, Li N, Yuan S, Zhou X, Ding F, Rao K, Ma M, Wang Z. A comparison of endocrine disruption potential of nonylphenol ethoxylate, vanillin ethoxylate, 4-n-nonylphenol and vanillin in vitro. Ecotoxicol Environ Saf. 2019 Jul 15;175:208-214. doi: 10.1016/j.ecoenv.2019.03.060. Epub 2019 Mar 19. PMID: 30901638.

In vivo study

1. Zalko D, Costagliola R, Dorio C, Rathahao E, Cravedi JP. In vivo metabolic fate of the xeno-estrogen 4-n-nonylphenol in Wistar rats. Drug Metab Dispos. 2003 Feb;31(2):168-78. doi: 10.1124/dmd.31.2.168. PMID: 12527697.

2. Hsieh CY, Miaw CL, Hsieh CC, Tseng HC, Yang YH, Yen CH. Effects of chronic 4-n-nonylphenol treatment on aortic vasoconstriction and vasorelaxation in rats. Arch Toxicol. 2009 Oct;83(10):941-6. doi: 10.1007/s00204-009-0447-6. Epub 2009 Jun 17. PMID: 19533100.

7. Bioactivity

Biological target:

Nonylphenol has been found to act as an agonist of the GPER (GPR30).

In vitro activity

In this study, the effects of NPEO, VAEO, 4-n-NP and Vanillin on the estrogen receptor α (ERα), androgen receptor (AR), thyroid hormone receptor (TR), retinoic X receptor β (RXRβ) and estrogen-related receptor γ (ERRγ) were determined and compared using a battery of recombined yeast strains expressing β-galactosidase. The results showed that NPEO and 4-n-NP acted as significant antagonists of ER, AR, TR and ERRγ. In addition, 4-n-NP also had antagonistic activity toward RXRβ. The in vitro data indicated that NPEO, 4-n-NP and VAEO have the potential to act as endocrine disruptors involving more than one nuclear hormone receptor.

Reference: Ecotoxicol Environ Saf. 2019 Jul 15;175:208-214. https://pubmed.ncbi.nlm.nih.gov/30901638/

In vivo activity

After a 20-week 4-n-NP treatment orally at the dosage of 10 and 50 muM in the drinking water, phenylephrine- and potassium chloride-induced concentration-dependent responsiveness assessed by wire myograph were both significantly higher in aorta isolated from 4-n-NP-treated rats compared with control rats, but acetylcholine-induced vasorelaxation was similar between these two groups. In addition, systemic oxidative stress and vascular, but not intestinal, oxidant enzyme activities assessed by lucigenin-amplified chemiluminescence were all markedly higher in 4-n-NP-treated rats. In conclusion, the results suggested that chronic in vivo 4-n-NP exposure augments vascular contractile responsiveness through enhanced vascular oxidant enzyme activity.

Reference: Arch Toxicol. 2009 Oct;83(10):941-6. https://pubmed.ncbi.nlm.nih.gov/19533100/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.