PO Box 31126
Dayton, OH 45437
Tel: 937.252.2989 Fax: 937.258.3937
E-mail: info@exciton.com
www.exciton.com

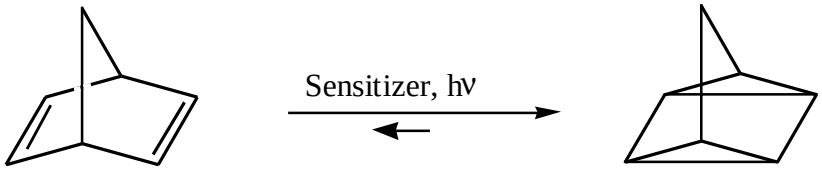
QUADRICYCLANE

Tetracyclo[3.2.0.0^{2,7}.0^{4,6}]heptane CASRN [278-06-8]

This unusual, highly strained molecule has found uses as a high energy rocket fuel and as a co-monomer in polymers for photolithography and optical data recording. The compound is now available for sale in quantities from 25 grams to > 25 kg.

Technical Information:

Quadricyclane is prepared by UV-irradiation of a sensitized solution of norbornadiene, either with a solvent such as diethyl ether[1], or neat. Conversions of up to about 99% are possible; Exciton offers 96.0% purity material by GC. Impurities include those retained from the starting norbornadiene, such as C_{12} and C_{14} components from the reaction of cyclopentadiene with norbornadiene and/or norbornadiene itself, norbornadiene, and toluene, the aromatic isomer of these C_7H_8 hydrocarbons.



(Photostationary
State is sensitizer-dependent)

Property	Norbornadiene	Quadricyclane
♦ Ionization Potential:	8.69	8.56
♦ Boiling Point:	89.5°C	108-111 °C
♦ Density:	0.9064	0.982
♦ Flash Point:	-11°C	+2°C
♦ Freezing Point:	-19°C	-44°C
♦ Increase in heat of combustion:		+110 kJ/mol (1200J/g)

Shipping and Hazard Information:

Packing Group I, UN3384, Toxic by Inhalation Liquid, Flammable, n.o.s. (quadricyclane), Hazard Zone B, LC_{50} (rat, 4 hours) 0.78 mg/L = 206 ppm (mL of vapor per m^3). [2]

References:

1. C. D. Smith, *Organic Syntheses, Coll. Vol. 6*, p. 962, 1988; *Vol. 51*, p. 133 (1971); http://www.orgsyn.org/orgsyn/orgsyn/prepContent.asp?prep=cv6p0962

2. Wolfe, R. E.; Kinkead, E. R.; Feldman, M. L.; Leahy, H. F.; Narayanan, L; Eggers, J. S., *Acute, Subchronic and Reproductive Toxicity of Quadricyclane Vapor on Sprague-Dawley Rats,* TR-1996-0128, AL/OE, Mantech Environmental Technology, Inc., Dayton, OH, Aug 1996.

Please inquire for pricing and availability.