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## Typical Product Specifications & Properties

# 1,6-Heptadiyne

CAS Number: : 2396-63-6

Specifications	Limits
Molecular weight	92.14
EINECS	219-253-5
SMILES	C#CCCCC#C
InChI	1S/C7H8/c1-3-5-7-6-4-2/h1-2H,5-7H2
InChIKey	RSPZSDWVQWRAEF-UHFFFAOYSA-N
Henry's Law Constant	6.18E-03 atm-m <sup>3</sup> /mole
Boiling Point	112 &deg; C
Water solubility	1650 mg/L
Atmospheric OH Rate Constant	1.77E-11 cm <sup>3</sup> /molecule-sec
Vapor Pressure	25.3 mm Hg
Melting Point	-8.50E+01 &deg; C
log P (octanol-water)	2.240



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Specifications	Limits
BRN Number	1731756
Storage Temperature	Refrigerator (+4&deg;C)
Water solubility	Insoluble in water.
Flash Point	49 &deg;F
Refractive Index	1.441
Boiling Point	111.5 &deg;C
Melting Point	-85 &deg;C
Density	0.805 g/mL at 25 &deg;C



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