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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-m3/mole
Boiling Point	112 ° C
Water solubility	1650 mg/L
Atmospheric OH Rate Constant	1.77E-11 cm3/molecule-sec
Vapor Pressure	25.3 mm Hg
Melting Point	-8.50E+01 ° C
log P (octanol-water)	2.240



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



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