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Typical Product Specifications & Properties

1-Heptyne

CAS Number: : 628-71-7

Specifications	Limits
Molecular weight	96.17
SMILES	C(CCC)CC#C
InChI	1S/C7H12/c1-3-5-7-6-4-2/h1H,4-7H2,2H3
InChIKey	YVXHZKKCZYLQOP-UHFFFAOYSA-N
Vapor Pressure	52.5 mm Hg
Water solubility	94 mg/L
Atmospheric OH Rate Constant	1.23E-11 cm ³ /molecule-sec
Melting Point	-8.10E+01 ° C
Boiling Point	99.7 ° C
log P (octanol-water)	3.010
Henry's Law Constant	0.071 atm-m ³ /mole



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