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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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