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Typical Product Specifications & Properties

2,6-Dimethyl-2,5-Heptadien-4-One

CAS Number: : 504-20-1

Specifications	Limits
Molecular weight	138.21
EINECS	207-986-3
SMILES	<chem>C(\C(\C=C(\C)C)=O)=C(/C)C</chem>
InChI	1S/C9H14O/c1-7(2)5-9(10)6-8(3)4/h5-6H,1-4H3
InChIKey	MTZWHHIREPJPTG-UHFFFAOYSA-N
Melting Point	28 ° C
Boiling Point	197.5 ° C
Atmospheric OH Rate Constant	6.14E-11 cm ³ /molecule-sec
Henry's Law Constant	8.31E-05 atm-m ³ /mole
Water solubility	436 mg/L
log P (octanol-water)	2.680
Vapor Density	4.8



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Specifications	Limits
Density	0.885 g/mL at 25 °C
Vapor Pressure	0.38 mm Hg (20 °C)
Refractive Index	1.497
Boiling Point	198-199 °C
Merck	7333
Flash Point	175 °F
Melting Point	23-26 °C



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