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Typical Product Specifications & Properties

1-Isopentylbenzene

CAS Number: : 2049-94-7

Specifications	Limits
Molecular weight	148.24
EINECS	218-075-5
SMILES	<chem>c1(CCC(C)C)ccccc1</chem>
InChI	1S/C11H16/c1-10(2)8-9-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InChIKey	XNXIYYFOYIUJIW-UHFFFAOYSA-N
log P (octanol-water)	4.430
Boiling Point	195 ° C
Atmospheric OH Rate Constant	1.01E-11 cm ³ /molecule-sec
Storage Temperature	Store below +30°C.
Flash Point	65 °C
Boiling Point	197 °C
Density	0.854 g/mL at 20 °C



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