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Typical Product Specifications & Properties

HSDB 5789

CAS Number: : 1119-40-0

Specifications	Limits
log P (octanol-water)	0.62
Water solubility	5.90E+04 mg/L
Henry's Law Constant	6.43E-07 atm-m ³ /mole
Boiling Point	214 ° C
Atmospheric OH Rate Constant	3.30E-12 cm ³ /molecule-sec
Melting Point	-4.25E+01 ° C
BRN Number	1771444
Melting Point	-13 ° C
Storage Temperature	2-8°C
Boiling Point	96-103 ° C/15 mm Hg
Merck	14&4473
Stability	Stable. Combustible. Incompatible with acids & bases & reducing agents & oxidizing agents.



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Specifications	Limits
Water solubility	53 g/L
Density	1.09 g/mL at 25 °C
Refractive Index	1.424
Flash Point	218 °F
Freezing Point	-42.5?
Vapor Pressure	0.2 mm Hg (20 °C)
EINECS	214-277-2
Molecular weight	160.1678
SMILES	<chem>C(=O)(CCCC(=O)OC)OC</chem>
InChIKey	1S/C7H12O4/c1-10-6(8)4-3-5-7(9)11-2/h3-5H2&1-2H3
InChI	XTDYIOOONNVFMA-UHFFFAOYSA-N



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