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Typical Product Specifications & Properties

Methylbenzethonium Chloride

CAS Number: : 25155-18-4

Specifications	Limits
Molecular weight	462.11
EINECS	246-675-7
SMILES	<chem>c1(ccc(OCCOCC[N+](Cc2ccccc2)(C)C)cc1)C(CC(C)(C)C)(C)C.[Cl-].*C</chem>
Merck	13,6051
Molecular weight	94.94
EINECS	200-813-2
SMILES	CBr
InChI	1S/CH3Br/c1-2/h1H3
InChIKey	GZUXJHMPEANEGY-UHFFFAOYSA-N
log P (octanol-water)	1.19
Atmospheric OH Rate Constant	4.02E-14 cm ³ /molecule-sec
Water solubility	1.52E+04 mg/L



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Specifications	Limits
Melting Point	-9.37E+01 ° C
Henry's Law Constant	0.00734 atm-m ³ /mole
Boiling Point	3.5 ° C
Vapor Pressure	1620 mm Hg
Boiling Point	4 °C
Storage Temperature	2-8°C
Melting Point	-94 °C
Refractive Index	1.4432
Water solubility	1.522 g/100 mL
Vapor Pressure	1420 mm Hg (20 °C)
Stability	Stable. Incompatible with oxidizing agents, strong acids. This is an ozone-depleting chemical, and its use is restricted in many countries.
Merck	13,6056



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Specifications	Limits
Flash Point	-34 °C
Density	3.3 g/mL at 25 °C
Vapor Density	3.3 (20 °C, vs air)



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