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Typical Product Specifications & Properties

3-(Trifluoromethyl)benzaldehyde

CAS Number: : 454-89-7

Specifications	Limits
Molecular weight	174.12
SMILES	<chem>O=Cc1cccc(C(F)(F)F)c1</chem>
InChI	1S/C8H5F3O/c9-8(10,11)7-3-1-2-6(4-7)5-12/h1-5H
InChIKey	NMTUHPSKJJYGML-UHFFFAOYSA-N
Water solubility	457 mg/L
log P (octanol-water)	2.47
Vapor Pressure	0.677 mm Hg
Atmospheric OH Rate Constant	1.70E-11 cm ³ /molecule-sec
Henry's Law Constant	1.17E-04 atm-m ³ /mole



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