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Typical Product Specifications & Properties

2-(Trifluoromethyl)benzoic acid

CAS Number: : 433-97-6

Specifications	Limits
Molecular weight	190.12
SMILES	<chem>c1(c(C(O)=O)cccc1)C(F)(F)F</chem>
InChI	1S/C8H5F3O2/c9-8(10,11)6-4-2-1-3-5(6)7(12)13/h1-4H,(H,12,13)
InChIKey	FBRJYBGLCHWYOE-UHFFFAOYSA-N
log P (octanol-water)	2.490
Water solubility	4800 mg/L
Melting Point	111 ° C
Atmospheric OH Rate Constant	6.29E-13 cm ³ /molecule-sec



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