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Typical Product Specifications & Properties

3-(Trifluoromethyl)benzoic acid

CAS Number: : 454-92-2

Specifications	Limits
Molecular weight	190.12
EINECS	207-230-2
SMILES	<chem>c1(cc(ccc1)C(O)=O)C(F)(F)F</chem>
InChI	1S/C8H5F3O2/c9-8(10,11)6-3-1-2-5(4-6)7(12)13/h1-4H,(H,12,13)
InChIKey	FQXQBFIUUVCDIRK-UHFFFAOYSA-N
Vapor Pressure	9.87E-03 mm Hg
Boiling Point	238.5 ° C
log P (octanol-water)	2.95
Henry's Law Constant	9.42E-07 atm-m3/mole
Atmospheric OH Rate Constant	6.65E-13 cm3/molecule-sec
Water solubility	149 mg/L
Melting Point	105.5 ° C



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Specifications	Limits
Boiling Point	238.5 °C/775 mm Hg
BRN Number	2049239
Flash Point	237-240°C
Melting Point	104-106 °C



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