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Typical Product Specifications & Properties

Floctafenine

CAS Number: : 23779-99-9

Specifications	Limits
Molecular weight	406.36
EINECS	245-881-4
SMILES	<chem>c12c(c(Nc3c(C(OC[C@@H](CO)O)=O)cccc3)ccn2)cccc1C(F)(F)F</chem>
InChI	1S/C20H17F3N2O4/c21-20(22,23)15-6-3-5-13-17(8-9-24-18(13)15)25-16-7-2-1-4-14(16)19(28)29-11-12(27)10-26/h1-9,12,26-27H,10-11H2,(H,24,25)
InChIKey	APQPGQGAWABJLN-UHFFFAOYSA-N
Atmospheric OH Rate Constant	9.17E-11 cm ³ /molecule-sec
log P (octanol-water)	3.980
Melting Point	179.5 °C



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415 Huguenot Street, New Rochelle, New York 10801

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