



www.parchem.com

Typical Product Specifications & Properties

(S)-9,10-Difluoro-3-methyl-7-oxo-2,3-dihydro-7H-pyrido[1,2,3-de][1,4]benzoxazine-6-carboxylic acid

CAS Number: : 100986-89-8

Specifications	Limits
Molecular weight	281.21
SMILES	<chem>C[C@H]1COc2c3n1cc(c(=O)c3cc(c2F)F)C(=O)O</chem>
InChI	NVKWWNNJFKZ NJO-YFKPBYRVSA-N
InChIKey	1S/C13H9F2NO4/c1-5-4-20-12-9(15)8(14)2-6-10(12)16(5)3-7(11(6)17)13(18)19/h2-3,5H,4H2,1H3,(H,18,19)/t5-/m0/s1
Melting Point	>300 °C
Storage Temperature	Refrigerator
Molecular weight	250.25
EINECS	202-966-0
SMILES	<chem>c1cc(ccc1Cc2ccc(cc2)N=C=O)N=C=O</chem>
InChI	1S/C15H10N2O2/c18-10-16-14-5-1-12(2-6-14)9-13-3-7-15(8-4-13)17-11-19/h1-8H,9H2
InChIKey	UPMLOUAZCHDJJD-UHFFFAOYSA-N
Flash Point	196 °C





www.parchem.com



GIVE US A CALL
800-282-3982
914-654-6800

GET A QUICK QUOTE

Specifications	Limits
Boiling Point	392 °C
Density	1.19
Melting Point	38-44 °C
BRN Number	797662
Water solubility	decomposes
Stability	Stable. Combustible. Incompatible with strong oxidizing agents. Reacts violently with alcohols.
Sensitive	Moisture Sensitive/Lachrymatory
Freezing Point	37?
Storage Temperature	Refrigerator
Freezing Point	37?
Vapor Pressure	5.00E-06 mm Hg
Henry's Law Constant	8.95E-07 atm-m3/mole



GET A QUICK QUOTE

415 Huguenot Street, New Rochelle, New York 10801

Disclaimer: this is a web generated product specification and property document. All information on this document is subject to reconfirmation at time of quote and order.



www.parchem.com



GIVE US A CALL
800-282-3982
914-654-6800

GET A QUICK QUOTE

Specifications	Limits
Melting Point	38 ° C
log P (octanol-water)	5.220
Water solubility	0.829 mg/L
Atmospheric OH Rate Constant	1.20E-11 cm ³ /molecule-sec
Freezing Point	37?



GET A QUICK QUOTE

415 Huguenot Street, New Rochelle, New York 10801

Disclaimer: this is a web generated product specification and property document. All information on this document is subject to reconfirmation at time of quote and order.