



www.parchem.com

## Typical Product Specifications & Properties

# 3-[(Prop-1-en-2-yl) phenyl] prop-2-yl isocyanate

CAS Number: : 2094-99-7

Specifications	Limits
Molecular weight	201.26
EINECS	402-440-2
SMILES	<chem>CC(=C)c1cccc(c1)C(C)(C)N=C=O</chem>
InChI	1S/C13H15NO/c1-10(2)11-6-5-7-12(8-11)13(3,4)14-9-15/h5-8H,1H2,2-4H3
InChIKey	ZVEMLYIXBCTVOF-UHFFFAOYSA-N
Boiling Point	268-271 °C
Density	1.018 g/mL at 25 °C
Flash Point	>230 °F
Refractive Index	1.53
Boiling Point	269.5 °C
Vapor Pressure	2.07E-04 mm Hg
Atmospheric OH Rate Constant	5.35E-11 cm <sup>3</sup> /molecule-sec



GET A QUICK QUOTE

415 Huguenot Street, New Rochelle, New York 10801



www.parchem.com



**parchem**  
fine & specialty chemicals

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

GET A QUICK QUOTE

Specifications	Limits
Henry's Law Constant	2.01E-06 atm-m <sup>3</sup> /mole
Water solubility	4.690 mg/L
log P (octanol-water)	4.640



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.