



www.parchem.com

## Typical Product Specifications & Properties

# NNC 0640

CAS Number: : 307986-98-7

Specifications	Limits
Canonicalized Compound	1
Compound Complexity	970
Hydrogen Bond Acceptor Count	7
Hydrogen Bond Donor Count	3
Rotatable Bond Count	8
Allowed IUPAC Name	4-[[4-cyclohexyl-N-[(3-methylsulfonylphenyl)carbamoyl]anilino]methyl]-N-(2H-tetrazol-5-yl)benzamide
CAS-like Style IUPAC Name	4-[(4-cyclohexyl-N-[(3-methylsulfonylanilino)-oxomethyl]anilino)methyl]-N-(2H-tetrazol-5-yl)benzamide
Markup IUPAC Name	4-[[4-cyclohexyl- $\langle \text{I} \rangle \text{N} \langle \text{I} \rangle$ -(3-methylsulfonylphenyl)carbamoyl]anilino]methyl]- $\langle \text{I} \rangle \text{N} \langle \text{I} \rangle$ -(2 $\langle \text{I} \rangle \text{H} \langle \text{I} \rangle$ -tetrazol-5-yl)benzamide
Preferred IUPAC Name	4-[[4-cyclohexyl-N-[(3-methylsulfonylphenyl)carbamoyl]anilino]methyl]-N-(2H-tetrazol-5-yl)benzamide
Systematic IUPAC Name	4-[[[(4-cyclohexylphenyl)-[(3-methylsulfonylphenyl)carbamoyl]amino]methyl]-N-(2H-1,2,3,4-tetrazol-5-yl)benzamide
Traditional IUPAC Name	4-[[4-cyclohexyl-N-[(3-methylsulfonylphenyl)carbamoyl]anilino]methyl]-N-(2H-tetrazol-5-yl)benzamide

GET A QUICK QUOTE

Standard InChI

InChI=1S/C29H31N7O4S/c1-41(39,40)26-9-5-8-24(18-26)30-29(38)36(25-16-14-22(15-17-25)31-6-3-24-7-21)19-20]10-12-23(13-11-20)27(37)31-28-32-34-35-33-28/h5,8-18,21H,2-4,6-7,19H2,1H3,(H,30,38)(H2,31,32,33,34,35,37)

415 Huguenot Street, New Rochelle, New York 10801



GET A QUICK QUOTE

Polar Surface Area	158
Topological Polar Surface Area	158
Monoisotopic Weight	573

415 Huguenot Street, New Rochelle, New York 10801

Weight: 575.21362507

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

Chemical  
Structure



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

GET A QUICK QUOTE



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.