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Typical Product Specifications & Properties

2-[2,4-bis(tert-pentyl)phenoxy]-N-[4-[4,5-dihydro-5-oxo-4-[(1-phenyl-1H-tetrazol-5-yl)thio]-3-(pyrro

CAS Number: : 30818-18-9

Specifications	Limits
Molecular weight	722.94
EINECS	250-348-4
SMILES	<chem>C([C@H])(CC)Oc1c(cc(cc1)C(CC)(C)C)C(CC)(C)C(=O)Nc1ccc(cc1)N1N=C([C@H](C1=O)Sc1nnnn1c1cccc1)N1CCCC1</chem>
InChI	XBRACQJIEMMORN-UHFFFAOYSA-N
InChIKey	1S/C40H50N8O3S/c1-8-32(51-33-23-18-27(39(4,5)9-2)26-31(33)40(6,7)10-3)36(49)41-28-19-21-30(22-20-28)47-37(50)34(35(43-47)46-24-14-15-25-46)52-38-42-44-45-48(38)29-16-12-11-13-17-29/h11-13,16-23,26,32,34H,8-10,14-15,24-25H2,1-7H3,(H,41,49)

