



www.parchem.com

Typical Product Specifications & Properties

1-(2-methylpropyl) 3-[(4-amino-9,10-dihydro-9,10-dioxo-3-sulpho-1-anthryl)amino]benzoate

CAS Number: : 85455-38-5

Specifications	Limits
Molecular weight	494.52
EINECS	287-273-1
SMILES	<chem>c12c(C(=O)c3c(C1=O)cccc3)c(cc(S(=O)(=O)O)c2N)Nc1cc(c(C(=O)O)cc1)CC(C)C</chem>
InChI	BPAZ AQGUFUHASG-UHFFFAOYSA-N
InChIKey	1S/C25H22N2O7S/c1-12(2)9-13-10-14(7-8-15(13)25(30)31)27-18-11-19(35(32,33)34)22(26)21-20(18)23(28)16-5-3-4-6-17(16)24(21)29/h3-8,10-12,27H,9,26H2,1-2H3,(H,30,31)(H,32,33,34)

