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## Typical Product Specifications & Properties

# Daigremontianin

CAS Number: : 98205-50-6

Specifications	Limits
SMILES	<chem>C(\c1c(cccc1)S(=O)(=O)[O-]) (c1ccc(N(Cc2cc(ccc2)S(=O)(=O) [O-])CC)cc1)=C1\C=C\C(=[N+](\Cc2cc(ccc2)S(=O)(=O) [O-])CC)C=C1.[NH4+].[NH4+]</chem>
InChI	HMEKVHWROSNWPD-UHFFFAOYSA-N
InChIKey	1S/C37H36N2O9S3.2H3N/c1-3-38(25-27-9-7-11-33(23-27)49(40,41)42)31-19-15-29(16-20-31)37(35-13-5-6-14-36(35)51(46,47)48)30-17-21-32(22-18-30)39(4-2)26-28-10-8-12-34(24-28)50(43,44)45;;/h5-24H,3-4,25-26H2,1-2H3,(H2-,40,41,42,43,44,45,46,47,48);2*1H3



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