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Typical Product Specifications & Properties

Dequalinium Acetate

CAS Number: : 4028-98-2

Specifications	Limits
Molecular weight	574.75
EINECS	223-712-5
SMILES	<chem>c12[n+](c(cc(c1cccc2)N)C)CCCCCCCCC[n+]1c2c(c(N)cc1C)ccc[O-].CC(=O)[O-]</chem>
InChI	IWYNVAJACBPVLT-UHFFFAOYSA-N
InChIKey	1S/C30H38N4.2C2H4O2/c1-23-21-27(31)25-15-9-11-17-29(25)33-7-5-3-4-6-8-14-20-34-24(2)22-28(32)26-16-10-12-18-30(26)34;2*1-12,15-18,21-22,31-32H,3-8,13-14,19-20H2,1-2H3;2*1H3,(H,3,4)



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