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Typical Product Specifications & Properties

Bisdequalinium Diacetate

CAS Number: : 3785-44-2

Specifications	Limits
Molecular weight	1,031.42
EINECS	223-252-5
SMILES	<chem>[n+]12c3c(cccc3)c(cc2C)NCCCCCCCCCNc2cc(C)[n+](CCCCCCCCC1)c1c2cccc1.[O-]C(C)=O.[O-]C(C)=O</chem>
InChI	GCWKUHNKKWYKOP-BGRABRFLSA-N
InChIKey	1S/C40H56N4.2C2H4O2/c1-33-31-37-35-23-15-17-25-39(35)43(33)29-21-13-9-5-6-10-14-22-30-44-34(2)32-38(36-24-16-18-26-40(36)44)42-28-20-12-8-4-3-7-11-19-27-41-37;2*1-2(3)4/h15-18,23-26,31-32H,3-14,19-22,27-30H2,1-2H3;2*1H3,(H,3,4)/b41-37+,42-38+;;



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