

data_compound1
_audit_creation_method 'WinGX routine-INITIALISE'
_audit_creation_date 2006-11-09T16:09:13-00:00
loop_
 _atom_type_symbol
 _atom_type_number_in_cell
C 34
H 48
O 10
 _cell_length_a 7.2710(2)
 _cell_length_b 9.6910(3)
 _cell_length_c 11.7480(4)
 _cell_angle_alpha 90
 _cell_angle_beta 93.725(1)
 _cell_angle_gamma 90
 _cell_formula_units_Z 2
 _cell_measurement_temperature 298
 _cell_measurement_wavelength 0.71073
 _cell_measurement_reflns_used 1840
 _cell_measurement_theta_max 27.485
 _cell_measurement_theta_min 3.395
 _diffrn_ambient_temperature 298
 _diffrn_radiation_probe x-ray
 _exptl_crystal_description prism
 _exptl_crystal_colour colourless
 _exptl_crystal_size_max 0.40
 _exptl_crystal_size_mid 0.36
 _exptl_crystal_size_min 0.18
 _exptl_crystal_density_method 'not measured'
 _chemical_formula_moiety 'C17 H24 O5'
 _chemical_formula_sum 'C17 H24 O5'
 _chemical_compound_source 'natural product as described'
 _symmetry_cell_setting monoclinic
 _symmetry_space_group_name_H-M 'P 1 21 1'
 _symmetry_space_group_name_Hall 'P 2yb'
 _symmetry_Int_Tables_number 4
 _computing_data_collection 'Collect (Nonius BV, 1997-2000)'
 _computing_cell_refinement
 'HKL Scalepack (Otwinowski & Minor 1997)'
 _computing_data_reduction
 'HKL Denzo and Scalepack (Otwinowski & Minor 1997)'
 _computing_structure_solution 'SHELXS-97 (Sheldrick, 1997)'
 _computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
 _computing_molecular_graphics 'Ortep-3 for Windows (Farrugia, 1997)'
 _computing_publication_material
'WinGX publication routines (Farrugia, 1999)'