

data_24d

_publ_contact_author_name 'Leslaw Sieron'
_publ_contact_author_email 'lsieron@p.lodz.pl'

loop_

_publ_author_name

"L.Sieron"

"J.Kobylecka"

"A.Turek"

_chemical_name_systematic '2,4-Dichlorophenoxy acetic acid'

_chemical_name_common '2,4-D'

_chemical_melting_point 414

_chemical_formula_moiety 'C8 H6 Cl2 O3'

_chemical_formula_sum 'C8 H6 Cl2 O3'

_chemical_formula_weight 221.03

_symmetry_cell_setting triclinic

_symmetry_space_group_name_Hall '-P 1'

_symmetry_space_group_name_H-M 'P -1'

_symmetry_Int_Tables_number 2

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_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

2 -x,-y,-z

_cell_length_a 7.1246(2)

_cell_length_b 7.8399(2)

_cell_length_c 8.8991(2)

_cell_angle_alpha 90.654(1)

_cell_angle_beta 104.565(1)

_cell_angle_gamma 110.527(1)

_cell_volume 447.82(2)

_cell_formula_units_Z 2

_cell_measurement_temperature 90

_exptl_crystal_colour 'colorless'

_exptl_crystal_preparation 'toluene'

_exptl_crystal_density_diffn 1.639

_exptl_crystal_F_000 224

_exptl_absorpt_coefficient_mu 0.692

_exptl_special_details 'herbicidal agent'

_diffn_ambient_temperature 90

_diffn_radiation_wavelength 0.71073

_diffn_radiation_probe 'x-ray'