

data_24db

_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-Dichlorophenoxybutanoic acid'

_chemical_name_common '2,4-DB'

_chemical_formula_moiety 'C10 H10 Cl2 O3'

_chemical_formula_sum 'C10 H10 Cl2 O3'

_chemical_formula_weight 249.08

_symmetry_cell_setting triclinic

_symmetry_space_group_name_Hall '-P 1'

_symmetry_space_group_name_H-M 'P -1'

_symmetry_Int_Tables_number 2

loop_

_symmetry_equiv_pos_site_id

_symmetry_equiv_pos_as_xyz

1 x,y,z

2 -x,-y,-z

_cell_length_a 7.4845(4)

_cell_length_b 8.7892(5)

_cell_length_c 9.3777(4)

_cell_angle_alpha 81.0720(14)

_cell_angle_beta 69.5538(13)

_cell_angle_gamma 65.3163(12)

_cell_volume 525.18(5)

_cell_formula_units_Z 2

_cell_measurement_temperature 90

_exptl_crystal_colour 'colorless'

_exptl_crystal_preparation 'toluene'

_exptl_crystal_density_diffn 1.575

_exptl_crystal_F_000 256

_exptl_absorpt_coefficient_mu 0.600

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_diffn_ambient_temperature 90

_diffn_radiation_wavelength 0.71073

_diffn_radiation_probe 'x-ray'