

Dimethylmalonic acid, 2,5-dichlorophenyl propyl ester

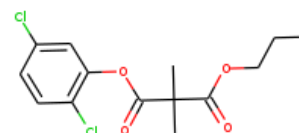
InChI: InChI=1S/C14H16Cl2O4/c1-4-7-19-12(17)14(2,3)13(18)20-11-8-9(15)5-6-10(11)16/h5-6,8H,4,7H2,1-3H3

InChI Key: NKOYRWAXUGHIP1-UHFFFAOYSA-N

Formula: C14H16Cl2O4

SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl

Molecular Weight: 319.18



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-328.71	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-648.53	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	31.83	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	76.14	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.88		Crippen Method
P_c	2021.76	kPa	Joback Method
T_{boil}	780.57	K	Joback Method
T_c	1003.61	K	Joback Method
T_{fus}	505.58	K	Joback Method
V_c	0.85	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	591.06	J/mol×K	780.57	Joback Method
η	0.00	Paxs	780.57	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H16Cl2O4/c1-4-7-19-12\(17\)14\(2,3\)13\(18\)20-11-8-9\(15\)5-6-10\(11\)16/h5-6,8H,4,7H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H16Cl2O4/c1-4-7-19-12(17)14(2,3)13(18)20-11-8-9(15)5-6-10(11)16/h5-6,8H,4,7H2,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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