

Dimethylmalonic acid, 2,3-dichlorophenyl isobutyl ester

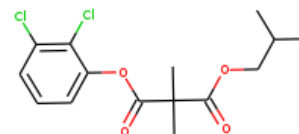
InChI: InChI=1S/C15H18Cl2O4/c1-9(2)8-20-13(18)15(3,4)14(19)21-11-7-5-6-10(16)12(11)17/h5-7,9H,8H2,1-4H3

InChI Key: RRZVLOVDSWMSGG-UHFFFAOYSA-N

Formula: C₁₅H₁₈Cl₂O₄

SMILES: CC(C)COC(=O)C(C)(C)C(=O)Oc1cccc(Cl)c1Cl

Molecular Weight: 333.21



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-322.73	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-674.45	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	30.90	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	77.98	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.12		Crippen Method
P_c	1870.79	kPa	Joback Method
T_{boil}	803.01	K	Joback Method
T_c	1026.59	K	Joback Method
T_{fus}	501.85	K	Joback Method
V_c	0.90	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	645.84	J/mol×K	803.01	Joback Method
η	0.00	Paxs	803.01	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H18Cl2O4/c1-9\(2\)8-20-13\(18\)15\(3,4\)14\(19\)21-11-7-5-6-10\(16\)12\(11\)17/h5-7,9H,8H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H18Cl2O4/c1-9(2)8-20-13(18)15(3,4)14(19)21-11-7-5-6-10(16)12(11)17/h5-7,9H,8H2,1-4H3)

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

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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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