

Diethylmalonic acid, 4-chloro-3-methylphenyl ethyl ester

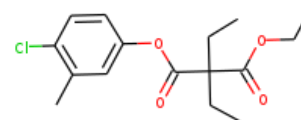
InChI: InChI=1S/C16H21ClO4/c1-5-16(6-2,14(18)20-7-3)15(19)21-12-8-9-13(17)11(4)10-12/h8-10H,5-7H2,1-4H3

InChI Key: RBSUHTKVPBQRHK-UHFFFAOYSA-N

Formula: C16H21ClO4

SMILES: CCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1

Molecular Weight: 312.79



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-299.94	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-674.07	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	32.82	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	76.21	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.923		Crippen Method
P_c	1766.90	kPa	Joback Method
T_{boil}	788.90	K	Joback Method
T_c	1003.50	K	Joback Method
T_{fus}	498.20	K	Joback Method
V_c	0.909	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	676.00	J/mol×K	788.9	Joback Method
η	0.0000671	Paxs	788.9	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H21ClO4/c1-5-16\(6-2,14\(18\)20-7-3\)15\(19\)21-12-8-9-13\(17\)11\(4\)10-12/h8-10H,5-7H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H21ClO4/c1-5-16(6-2,14(18)20-7-3)15(19)21-12-8-9-13(17)11(4)10-12/h8-10H,5-7H2,1-4H3)

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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