

Dichloroacetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl

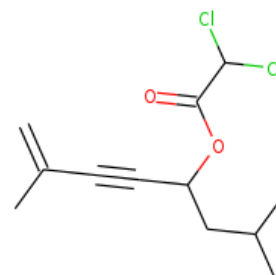
InChI: InChI=1S/C12H16Cl2O2/c1-8(2)5-6-10(7-9(3)4)16-12(15)11(13)14/h9-11H,1,7H2,2-4H3

InChI Key: VSXCBHKTNKYJJP-UHFFFAOYSA-N

Formula: C₁₂H₁₆Cl₂O₂

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)C(Cl)Cl

Molecular Weight: 263.16



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	67.15	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-195.19	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	27.98	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	60.63	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.33		Crippen Method
P_c	2129.52	kPa	Joback Method
T_{boil}	629.35	K	Joback Method
T_c	845.58	K	Joback Method
T_{fus}	402.38	K	Joback Method
V_c	0.76	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	465.05	J/mol×K	629.35	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16Cl2O2/c1-8\(2\)5-6-10\(7-9\(3\)4\)16-12\(15\)11\(13\)14/h9-11H,1,7H2,2-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16Cl2O2/c1-8(2)5-6-10(7-9(3)4)16-12(15)11(13)14/h9-11H,1,7H2,2-4H3)

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

Legend

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

$\Delta_f G^\circ$: 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).

$\log P_{oct/wat}$: 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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