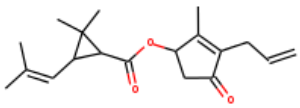
Bioallethrin



Other names: (.+/-.)-3-Allyl-2-methyl-4-oxocyclopent-2-enyl 2,2-dimethyl-3-(2-methylprop-1-enyl) cyclopropylcarboxylate; (.+/-.)-Allelrethonyl (.+/-.)-cis,trans-chrysanthemate; (RS)-3-Allyl-2-methyl-4-oxocyclopent-2-enyl (1R,3R)-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate; 2-Allyl-4-hydroxy-3-methyl-2-cyclopenten-1-one ester of 2,2-dimethyl-3-(2-methyl propenyl) cyclopropane carboxylic acid; 2-Methyl -4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl-2,2-dimethyl-3-(2-methyl-1-prop enyl)cyclopropanecarboxylate; 3-Allyl-2-methyl-4-oxo-2-cyclopenten-1-yl chrysanthemate; 3-Allyl-4-keto-2-methylcyclopentenyl chrysanthemum monocarboxylate; 3-Allyl-4-methyl-2-oxo-3-cyclopenten-1-yl ester of 2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylic acid; Allethrin; Allethrin-1; Allethrine; Alleviate; Allyl cinerin I; Allyl homolog of cinerin I; Bioaletrina; Chrysanthemummonocarboxylic acid, 3-allyl-3-methyl-4-oxo-2-cyclopenten-1-yl ester; Cinerin I allyl homolog; Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propen-1-yl)-, 2-methyl-4-oxo-3-(2-propen-1-yl)-2-cyclopenten-1-yl ester; Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl ester; Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl ester, d-trans-; Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-propenyl)-2-cyclopentene-1-yl ester; Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, ester with 2-allyl-4-hydroxy-3-methyl-2-cyclopenten-1-one; D,L-2-Allyl-4-hydroxy-3-methyl-2-cyclopenten-1-one-D,L-chrysanthemum monocarboxylate; ENT 16275; ENT 17510; Exthrin; FDA 1446; FMC 249; Matox; NIA 249; Necarboxylic acid; Pallethrine; Pynamin; Pynamin-forte; Pyresin; Pyresyn; Pyrethrin; RU 27436; dl-Allethrin; trans-Allethrin; trans-Bioallethrin.

InChI: InChI=1S/C19H26O3/c1-7-8-13-12(4)16(10-15(13)20)22-18(21)17-14(9-11(2)3)19(17,5)6/h7,9,14,16-17H,1,8,10H2,2-6H3

InChI Key: ZCVAOQKBXKSDMS-UHFFFAOYSA-N

Formula: C19H26O3

SMILES: C=CCC1=C(C)C(OC(=O)C2C(C=C(C)C)C2(C)C)CC1=O

Molecular Weight: 302.41

CAS: 584-79-2

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-0.81	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-442.45	kJ/mol	Joback Method
$\Delta_{fus} H°$	33.23	kJ/mol	Joback Method

Property	Value	Unit	Source
$\Delta_{vap}H°$	70.68	kJ/mol	Joback Method
$logP_{oct/wat}$	4.00		Crippen Method
P_c	1517.57	kPa	Joback Method
T_{boil}	800.99	K	Joback Method
T_c	1021.94	K	Joback Method
T_{fus}	493.53	K	Joback Method
V_c	0.97	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	792.44	J/mol×K	800.99	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H26O3/c1-7-8-13-12(4)16(10-15(13)20)22-18(21)17-14(9-11(2)3)19(17,5)6/h7,9,14,16-17H,1,8,10H2,2-6H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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 (m^3/kg-mol).