Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester, [1R-[1«alpha»[S*(Z)],3«beta»]]-

Other names:	(+)-Pyrethronyl (+)-trans-chrysanthemate
	Chrysanthemummonocarboxylic acid pyrethrolone ester
	Pyrethrin I
	Piretrina 1
	Pyrethrolone, chrysanthemum monocarboxylic acid ester
	Rcra waste number P008
	(1S)-2-Methyl-4-oxo-3-[(2Z)-2,4-pentadienyl]-2-cyclopenten-1-yl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate, (1R,3R)-
	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester
	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, ester with 4-hydroxy-3-methyl-2-(2,4-pentadienyl)-2-cyclopenten-1-one
	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, (1S)-2-methyl-4-oxo-3-(2Z)-2,4-pentadienyl-2-cyclopenten-1-yl ester, (1R,3R)-
	2-methyl-4-oxo-3-(penta-2,4-dienyl)cyclopent-2-enyl [1R-[1«alpha»[S*(Z)],3«beta»]]-chrysanthemate
Inchi:	InChI=1S/C21H28O3/c1-7-8-9-10-15-14(4)18(12-17(15)22)24-20(23)19-16(11-13(2)3)21
InchiKey:	ROVGZAWFACYCSP-HJWRWDBZSA-N
Formula:	C21H28O3
SMILES:	C=CC=CCC1=C(C)C(OC(=O)C2C(C=C(C)C)C2(C)C)CC1=O
Mol. weight [g/mol]:	328.45
CAS:	121-21-1

Physical Properties

Property code	Value	Unit	Source
gf	96.25	kJ/mol	Joback Method
hf	-366.51	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.558		Crippen Method
mcvol	276.840	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	850.91	K	Joback Method
tc	1073.70	K	Joback Method
tf	510.99	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.31	J/mol×K	850.91	Joback Method
cpg	906.77	J/mol×K	888.04	Joback Method
cpg	926.67	J/mol×K	925.17	Joback Method
cpg	946.18	J/mol×K	962.31	Joback Method
cpg	965.45	J/mol×K	999.44	Joback Method
cpg	984.64	J/mol×K	1036.57	Joback Method
cpg	1003.91	J/mol×K	1073.70	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume