Pyrethrin II

Other names:

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

Cyclopropaneacrylic acid, 3-carboxy-«alpha»,2,2-trimethyl-, 1-methyl ester, ester with 4-hydroxy-3-methyl-2-(2,4-pentadienyl)-2-cyclopenten-1-one

(+)-Pyrethronyl (+)-pyrethrate

Cyclopropanecarboxylic acid, 3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-2,2-dimethyl-, 2-methyl-4-oxo-3-(2,4-pentadienyl)-2-cyclopenten-1-yl ester

Pyrethrin

Pyrethrin 2

Chrysanthemumdicarboxylic acid monomethyl ester pyrethrolone ester

ENT 7,543

Pyrethrolone, chrysanthemum dicarboxlic acid methyl ester ester

Pyrethrolone ester of chrsanthemumdicarboxylic acid monomethyl ester

Pyretrin II

Biospray S

Cyclopropanecarboxylic acid, 3-[(1E)-3-methoxy-2-methyl-3-oxo-1-propenyl]-2,2-dimethyl-, (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»)-3-(3-methoxy-2-methyl-3-oxoprop-1-enyl)-2,2-dimethylcyc

Inchi: InChI=1S/C22H28O5/c1-7-8-9-10-15-14(3)18(12-17(15)23)27-21(25)19-16(22(19,4)5)11-

InchiKey: VJFUPGQZSXIULQ-VKTMSVCMSA-N

Formula: $C_{22}H_{28}O_5$

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

Mol. weight [g/mol]: 372.45

CAS: 121-29-9

Physical Properties

Property code	Value	Unit	Source
gf	-129.25	kJ/mol	Joback Method
hf	-631.95	kJ/mol	Joback Method
hfus	43.99	kJ/mol	Joback Method
hvap	86.47	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.711		Crippen Method
mcvol	298.370	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2629.00		NIST Webbook
tb	950.08	K	Joback Method
tc	1177.90	K	Joback Method
tf	594.42	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.78	J/mol×K	950.08	Joback Method
cpg	1018.67	J/mol×K	988.05	Joback Method
cpg	1038.21	J/mol×K	1026.02	Joback Method
cpg	1057.53	J/mol×K	1063.99	Joback Method
cpg	1076.79	J/mol×K	1101.96	Joback Method
cpg	1096.15	J/mol×K	1139.93	Joback Method
cpg	1115.75	J/mol×K	1177.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121299&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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