

# Pyrethrin II

<b>Other names:</b>	Cyclopropanecarboxylic acid, 3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-2,2-dimethyl- 5-cyclopropaneacrylic acid, 3-carboxy, «alpha»,2,2-trimethyl-, 1-methyl ester, ester with 4-hydroxy-3-methyl-[2-(2,4-pentadienyl)-2-cyclopenten-1-yl]ester [(1R)-Pyrethrin II] [(S)-(1R)-Pyrethrate (E)]
	Cyclopropanecarboxylic acid, 3-(3-methoxy-2-methyl-3-oxo-1-propenyl)-2,2-dimethyl- 5-cyclopropaneacrylic acid, 3-carboxy, «alpha»,2,2-trimethyl-, 1-methyl ester Pyrethrin 2
	Chrysanthemumdicarboxylic acid monomethyl ester pyrethrolone ester ENT 7,543
	Pyrethrolone, chrysanthemum dicarboxylic acid methyl ester ester
	Pyrethrolone ester of chrysanthemumdicarboxylic acid monomethyl ester
	Pyretrin II
	Biospray S
	Cyclopropanecarboxylic acid, 3-[{(1E)-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,3R)- [(1R)-3-methoxy-2-methyl-3-oxo-1-propenyl]-2,2-dimethyl-5-cyclopropaneacrylic acid, 3-carboxy, «alpha»,2,2-trimethyl-, 1-methyl ester, ester 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)
<b>Inchi:</b>	
<b>InchiKey:</b>	VJFUPGQZSXIUHQ-VKTMSVCMSA-N
<b>Formula:</b>	C22H28O5
<b>SMILES:</b>	C=CC=CCC1=C(C)C(OC(=O)C2C(C=C(C)C(=O)OC)C2(C)C)CC1=O
<b>Mol. weight [g/mol]:</b>	372.45
<b>CAS:</b>	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
rinp0l	2615.00		NIST Webbook
rinp0l	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

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

## 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
rinpolt:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

**vc:**

Critical Volume

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