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

Other names:	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, ester with 4-hydroxy-3-methyl-2-(2-pentenyl)-2-cyclopenten-1-one
	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, 2-methyl-4-oxo-3-(2-pentenyl)-2-cyclopenten-1-yl ester
	Jasmolin I
	Jasmoline I
	Pyrethrin (Jasmolin I)
Inchi:	InChI=1S/C21H30O3/c1-7-8-9-10-15-14(4)18(12-17(15)22)24-20(23)19-16(11-13(2)3)21
InchiKey:	NZKIRHFOLVYKFT-CMDGGOBGSA-N
Formula:	C21H30O3
SMILES:	CCC=CCC1=C(C)C(OC(=O)C2C(C=C(C)C)C2(C)C)CC1=O
Mol. weight [g/mol]:	330.46
CAS:	4466-14-2

Physical Properties

Property code	Value	Unit	Source
gf	8.41	kJ/mol	Joback Method
hf	-491.94	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	75.76	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.782		Crippen Method
mcvol	281.140	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
tb	854.23	K	Joback Method
tc	1074.28	K	Joback Method
tf	512.75	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.13	J/mol×K	854.23	Joback Method
cpg	935.02	J/mol×K	890.90	Joback Method
cpg	955.32	J/mol×K	927.58	Joback Method
cpg	975.18	J/mol×K	964.25	Joback Method

cpg	994.74	J/mol×K	1000.93	Joback Method
cpg	1014.16	J/mol×K	1037.60	Joback Method
cpg	1033.56	J/mol×K	1074.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4466142&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume