Ethyl chrysanthemate

Other names:	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)-, ethyl ester
	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)-, ethyl ester
	Ethyl chrysanthemumate
	Chrysanthemum-monocarboxlic acid ethyl ester
	2,2-Dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylic acid ethyl ester
	ethyl 2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate
Inchi:	InChI=1S/C12H20O2/c1-6-14-11(13)10-9(7-8(2)3)12(10,4)5/h7,9-10H,6H2,1-5H3
InchiKey:	VIMXTGUGWLAOFZ-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CCOC(=O)C1C(C=C(C)C)C1(C)C
Mol. weight [g/mol]:	196.29
CAS:	97-41-6

Physical Properties

Property code	Value	Unit	Source
gf	-72.25	kJ/mol	Joback Method
hf	-381.02	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	49.64	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.788		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	551.93	K	Joback Method
tc	750.39	K	Joback Method
tf	311.48	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.84	J/mol×K	551.93	Joback Method
cpg	449.74	J/mol×K	585.01	Joback Method
cpg	465.71	J/mol×K	618.08	Joback Method

cpg	480.85	J/mol×K	651.16	Joback Method
cpg	495.27	J/mol×K	684.24	Joback Method
cpg	509.05	J/mol×K	717.31	Joback Method
cpg	522.31	J/mol×K	750.39	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	1.30	NIST Webbook
tbrp	392.00 ± 1.00	K	2.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97416&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume