Chrysanthemic acid

Other names:	Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methyl-1-propenyl)- Cyclopropanecarboxylic acid, 2,2-dimethyl-3-(2-methylpropenyl)- (.+/-.)-Chrysanthemumic acid Chrysanthemumic acid Chrysanthemummonocarboxylic acid 2-(1-Isobutenyl)-3,3-dimethylcyclopropanecarboxylic acid 3-Isobutenyl-2,2-dimethylcyclopropanecarboxylic acid 2,2-Dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylic acid NSC 11779 Chrysantemic acid 2,2-Dimethyl-3-(2-methyl-1-propen-1-yl)cyclopropanecarboxylic acid (chrysanthemic acid)
Inchi:	InChI=1S/C10H16O2/c1-6(2)5-7-8(9(11)12)10(7,3)4/h5,7-8H,1-4H3,(H,11,12)
InchiKey:	XLOPRKKSAJMMEW-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)=CC1C(C(=O)O)C1(C)C
Mol. weight [g/mol]:	168.23
CAS:	10453-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-120.91	kJ/mol	Joback Method
hf	-359.75	kJ/mol	Joback Method
hfus	20.21	kJ/mol	Joback Method
hvap	59.46	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.309		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	1283.00		NIST Webbook
rinpol	1283.00		NIST Webbook
tb	575.93	K	Joback Method
tc	769.15	K	Joback Method
tf	327.53	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.33	J/mol×K	575.93	Joback Method
cpg	383.28	J/mol×K	608.13	Joback Method
cpg	395.50	J/mol×K	640.34	Joback Method
cpg	407.10	J/mol×K	672.54	Joback Method
cpg	418.17	J/mol×K	704.74	Joback Method
cpg	428.81	J/mol×K	736.94	Joback Method
cpg	439.13	J/mol×K	769.15	Joback Method
hfust	14.51	kJ/mol	390.70	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10453891&Units=SI

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
hfust: Enthalpy of fusion at a given temperature
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