Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, ethyl ester

Othernames: Ethyl 2-(2,2-dichlorovinyl)-3,3-dimethylcyclopropanecarboxylate
Ethyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-1-carboxylate
3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid, ethyl ester
Ethyl 3-(2,2-dichlorovinyl)-2,2-dimethyl-1-cyclopropanecarboxylate,c&t
ethyl 3-(2,2-dichlorovinyl)-2,2-dimethyl-1-cyclopropanecarboxylate

Inchi: InChI=1S/C10H14Cl2O2/c1-4-14-9(13)8-6(5-7(11)12)10(8,2)3/h5-6,8H,4H2,1-3H3

InchiKey: QPTWKDNRYCGMJM-UHFFFAOYSA-N

Formula: C10H14Cl2O2

SMILES: CCOC(=O)C1C(C=C(Cl)Cl)C1(C)C

Mol. weight [g/mol]: 237.12

CAS: 59609-49-3

Physical Properties

Property code	Value	Unit	Source
gf	-112.95	kJ/mol	Joback Method
hf	-371.22	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	53.96	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.141		Crippen Method
mcvol	168.520	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	581.03	K	Joback Method
tc	794.44	K	Joback Method
tf	348.78	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.66	J/mol×K	581.03	Joback Method
cpg	408.31	J/mol×K	616.60	Joback Method
cpg	421.15	J/mol×K	652.17	Joback Method
cpg	433.29	J/mol×K	687.74	Joback Method

cpg	444.85	J/mol×K	723.31	Joback Method
cpg	455.97	J/mol×K	758.87	Joback Method
cpg	466.75	J/mol×K	794.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.70	K	2.00	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=C59609493&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
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

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