Cyclopropanecarboxylic acid, 2,2-dichloro-1-methyl-, methyl ester

Other names: Methyl 2,2-dichloro-1-methylcyclopropanecarboxylate
Inchi: InChI=1S/C6H8Cl2O2/c1-5(4(9)10-2)3-6(5,7)8/h3H2,1-2H3
InchiKey: JGCAZFUFORGMFB-UHFFFAOYSA-N
Formula: C6H8Cl2O2
SMILES: COC(=O)C1(C)CC1(Cl)Cl
Mol. weight [g/mol]: 183.03
CAS: 1447-13-8

Physical Properties

Property code	Value	Unit	Source
gf	-216.08	kJ/mol	Joback Method
hf	-360.51	kJ/mol	Joback Method
hfus	9.09	kJ/mol	Joback Method
hvap	44.18	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.743		Crippen Method
mcvol	116.460	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	490.38	K	Joback Method
tc	713.66	K	Joback Method
tf	350.88	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.61	J/mol×K	490.38	Joback Method
cpg	245.46	J/mol×K	527.59	Joback Method
cpg	254.30	J/mol×K	564.81	Joback Method
cpg	262.34	J/mol×K	602.02	Joback Method
cpg	269.78	J/mol×K	639.23	Joback Method
cpg	276.85	J/mol×K	676.45	Joback Method
cpg	283.75	J/mol×K	713.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.20	K	1.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1447138&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