

2-Propenoic acid, 3-chloro-, methyl ester, (Z)-

Inchi:	InChI=1S/C4H5ClO2/c1-7-4(6)2-3-5/h2-3H,1H3/b3-2-
InchiKey:	ZLDNFLVIPPOXQL-IHWYPQMZSA-N
Formula:	C4H5ClO2
SMILES:	COC(=O)C=CCl
Mol. weight [g/mol]:	120.53
CAS:	3510-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-182.83	kJ/mol	Joback Method
hf	-269.21	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	38.00	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.912		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	408.80	K	Joback Method
tc	606.12	K	Joback Method
tf	231.84	K	Joback Method
vc	0.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.25	J/mol×K	408.80	Joback Method
cpg	164.07	J/mol×K	573.24	Joback Method
cpg	158.85	J/mol×K	540.35	Joback Method
cpg	153.36	J/mol×K	507.46	Joback Method
cpg	147.60	J/mol×K	474.57	Joback Method
cpg	141.57	J/mol×K	441.69	Joback Method
cpg	169.05	J/mol×K	606.12	Joback Method
dvisc	0.0002691	Pa×s	408.80	Joback Method
dvisc	0.0003383	Pa×s	379.31	Joback Method

dvisc	0.0004420	Pa×s	349.81	Joback Method
dvisc	0.0006066	Pa×s	320.32	Joback Method
dvisc	0.0008877	Pa×s	290.83	Joback Method
dvisc	0.0014158	Pa×s	261.33	Joback Method
dvisc	0.0025428	Pa×s	231.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3510449&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
dvisc:	Dynamic viscosity
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

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