Propanoic acid, 3-chloro, 1-methyl-3-butenyl ester

Inchi: InChI=1S/C8H13ClO2/c1-3-4-7(2)11-8(10)5-6-9/h3,7H,1,4-6H2,2H3
InchiKey: IVXMPKJYRQBPCG-UHFFFAOYSA-N
Formula: C8H13ClO2
SMILES: C=CCC(C)OC(=O)CCCl
Mol. weight [g/mol]: 176.64

Physical Properties

Property code	Value	Unit	Source
gf	-143.97	kJ/mol	Joback Method
hf	-348.84	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	45.89	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.123		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1102.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1596.00		NIST Webbook
tb	492.40	K	Joback Method
tc	680.78	K	Joback Method
tf	265.24	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	290.22	J/mol×K	492.40	Joback Method
cpg	301.76	J/mol×K	523.80	Joback Method
cpg	312.79	J/mol×K	555.19	Joback Method
cpg	323.33	J/mol×K	586.59	Joback Method
cpg	333.38	J/mol×K	617.98	Joback Method
cpg	342.95	J/mol×K	649.38	Joback Method
cpg	352.05	J/mol×K	680.78	Joback Method
dvisc	0.0039024	Pa×s	265.24	Joback Method
dvisc	0.0018579	Pa×s	303.10	Joback Method
dvisc	0.0010430	Pa×s	340.96	Joback Method
dvisc	0.0006571	Pa×s	378.82	Joback Method
dvisc	0.0004503	Pa×s	416.68	Joback Method
dvisc	0.0003286	Pa×s	454.54	Joback Method
dvisc	0.0002517	Pa×s	492.40	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R113830&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume