Butanoic acid, 2-chloro, 1-methyl-3-butenyl ester

Inchi: InChI=1S/C9H15ClO2/c1-4-6-7(3)12-9(11)8(10)5-2/h4,7-8H,1,5-6H2,2-3H3
InchiKey: XVIOVVXTFAHOIW-UHFFFAOYSA-N
Formula: C9H15ClO2
SMILES: C=CCC(C)OC(=O)C(Cl)CC
Mol. weight [g/mol]: 190.67

Physical Properties

Property code	Value	Unit	Source
gf	-137.99	kJ/mol	Joback Method
hf	-374.76	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.512		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1121.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1590.00		NIST Webbook
tb	514.84	K	Joback Method
tc	705.02	K	Joback Method
tf	261.51	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.17	J/mol×K	514.84	Joback Method
cpg	347.02	J/mol×K	546.54	Joback Method
cpg	359.28	J/mol×K	578.23	Joback Method

cpg	370.97	J/mol×K	609.93	Joback Method
cpg	382.09	J/mol×K	641.62	Joback Method
cpg	392.66	J/mol×K	673.32	Joback Method
cpg	402.69	J/mol×K	705.02	Joback Method
dvisc	0.0054436	Pa×s	261.51	Joback Method
dvisc	0.0021958	Pa×s	303.73	Joback Method
dvisc	0.0011055	Pa×s	345.95	Joback Method
dvisc	0.0006461	Pa×s	388.18	Joback Method
dvisc	0.0004196	Pa×s	430.40	Joback Method
dvisc	0.0002944	Pa×s	472.62	Joback Method
dvisc	0.0002189	Pa×s	514.84	Joback Method

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=R28572&Units=SI

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