Butanoic acid, 3-chloro, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C9H17ClO2/c1-6(2)8(4)12-9(11)5-7(3)10/h6-8H,5H2,1-4H3
InchiKey: VVRYCRWOHNYBFY-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CC(Cl)CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-228.27	kJ/mol	Joback Method
hf	-505.47	kJ/mol	Joback Method
hfus	15.48	kJ/mol	Joback Method
hvap	48.00	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.591		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1146.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1141.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	517.72	K	Joback Method
tc	708.11	K	Joback Method
tf	248.27	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.90	J/mol×K	517.72	Joback Method

cpg	366.71	J/mol×K	549.45	Joback Method
cpg	379.92	J/mol×K	581.18	Joback Method
cpg	392.53	J/mol×K	612.91	Joback Method
cpg	404.54	J/mol×K	644.64	Joback Method
cpg	415.98	J/mol×K	676.38	Joback Method
cpg	426.84	J/mol×K	708.11	Joback Method
dvisc	0.0089985	Pa×s	248.27	Joback Method
dvisc	0.0029439	Pa×s	293.18	Joback Method
dvisc	0.0012960	Pa×s	338.09	Joback Method
dvisc	0.0006916	Pa×s	383.00	Joback Method
dvisc	0.0004210	Pa×s	427.90	Joback Method
dvisc	0.0002817	Pa×s	472.81	Joback Method
dvisc	0.0002020	Pa×s	517.72	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28728&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