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

Inchi: InChI=1S/C9H17ClO2/c1-5-7(10)8(11)12-9(3,4)6-2/h7H,5-6H2,1-4H3
InchiKey: ITWMRGNRMHGDAZ-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCC(Cl)C(=O)OC(C)(C)CC
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-220.55	kJ/mol	Joback Method
hf	-503.66	kJ/mol	Joback Method
hfus	15.11	kJ/mol	Joback Method
hvap	47.48	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.736		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1107.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1103.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1402.00		NIST Webbook
tb	515.37	K	Joback Method
tc	709.03	K	Joback Method
tf	280.69	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.54	J/mol×K	515.37	Joback Method
cpg	369.63	J/mol×K	547.65	Joback Method
cpg	383.00	J/mol×K	579.92	Joback Method
cpg	395.67	J/mol×K	612.20	Joback Method
cpg	407.66	J/mol×K	644.48	Joback Method
cpg	418.99	J/mol×K	676.75	Joback Method
cpg	429.70	J/mol×K	709.03	Joback Method
dvisc	0.0053444	Pa×s	280.69	Joback Method
dvisc	0.0022594	Pa×s	319.80	Joback Method
dvisc	0.0011524	Pa×s	358.92	Joback Method
dvisc	0.0006709	Pa×s	398.03	Joback Method
dvisc	0.0004303	Pa×s	437.14	Joback Method
dvisc	0.0002969	Pa×s	476.26	Joback Method
dvisc	0.0002167	Pa×s	515.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28554&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
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