Butanoic acid, 2-chloro, 2-methylpropyl ester

Other names: Isobutyl 2-chlorobutyrate
Inchi: InChI=1S/C8H15ClO2/c1-4-7(9)8(10)11-5-6(2)3/h6-7H,4-5H2,1-3H3
InchiKey: YJVGEKBXSUEJIN-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CCC(Cl)C(=O)OCC(C)C
Mol. weight [g/mol]: 178.66
CAS: 22710-13-0

Physical Properties

Property code	Value	Unit	Source
chl	-4644.70	kJ/mol	NIST Webbook
chl	-4653.90 ± 8.40	kJ/mol	NIST Webbook
gf	-234.25	kJ/mol	Joback Method
hf	-609.20 ± 9.60	kJ/mol	NIST Webbook
hfl	-661.50 ± 8.40	kJ/mol	NIST Webbook
hfus	16.41	kJ/mol	Joback Method
hvap	52.30 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.203		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1069.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1403.00		NIST Webbook
tb	495.28	K	Joback Method
tc	683.89	K	Joback Method
tf	252.00	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.11	J/mol×K	495.28	Joback Method
cpg	320.63	J/mol×K	526.72	Joback Method
cpg	332.62	J/mol×K	558.15	Joback Method
cpg	344.09	J/mol×K	589.59	Joback Method
cpg	355.06	J/mol×K	621.02	Joback Method
cpg	365.51	J/mol×K	652.46	Joback Method
cpg	375.47	J/mol×K	683.89	Joback Method
dvisc	0.0061890	Pa×s	252.00	Joback Method
dvisc	0.0024580	Pa×s	292.55	Joback Method
dvisc	0.0012223	Pa×s	333.09	Joback Method
dvisc	0.0007073	Pa×s	373.64	Joback Method
dvisc	0.0004556	Pa×s	414.19	Joback Method
dvisc	0.0003174	Pa×s	454.73	Joback Method
dvisc	0.0002346	Pa×s	495.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22710130&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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