Butanoic acid, 2-chloro, 3-methylbutyl ester

Other names: 3-Methylbutyl 2-chlorobutyrate
Inchi: InChI=1S/C9H17ClO2/c1-4-8(10)9(11)12-6-5-7(2)3/h7-8H,4-6H2,1-3H3
InchiKey: WDSOYGRXTBCUIP-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCC(Cl)C(=O)OCCC(C)C
Mol. weight [g/mol]: 192.68
CAS: 62108-78-5

Physical Properties

Property code	Value	Unit	Source
chl	-5300.70	kJ/mol	NIST Webbook
chl	-5310.80 ± 8.40	kJ/mol	NIST Webbook
gf	-225.83	kJ/mol	Joback Method
hf	-630.10 ± 9.60	kJ/mol	NIST Webbook
hfl	-684.10 ± 8.40	kJ/mol	NIST Webbook
hfus	19.00	kJ/mol	Joback Method
hvap	54.00 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.593		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1173.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1503.00		NIST Webbook
tb	518.16	K	Joback Method
tc	704.64	K	Joback Method
tf	263.27	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.64	J/mol×K	518.16	Joback Method
cpg	414.29	J/mol×K	673.56	Joback Method
cpg	403.08	J/mol×K	642.48	Joback Method
cpg	391.31	J/mol×K	611.40	Joback Method
cpg	378.99	J/mol×K	580.32	Joback Method
cpg	366.10	J/mol×K	549.24	Joback Method
cpg	424.95	J/mol×K	704.64	Joback Method
dvisc	0.0002141	Pa×s	518.16	Joback Method
dvisc	0.0002907	Pa×s	475.68	Joback Method
dvisc	0.0004189	Pa×s	433.20	Joback Method
dvisc	0.0006537	Pa×s	390.72	Joback Method
dvisc	0.0011372	Pa×s	348.23	Joback Method
dvisc	0.0023072	Pa×s	305.75	Joback Method
dvisc	0.0058815	Pa×s	263.27	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=C62108785&Units=SI

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