Butanoic acid, 3-chloro, 1-methylpropyl ester

Inchi: InChI=1S/C8H15ClO2/c1-4-7(3)11-8(10)5-6(2)9/h6-7H,4-5H2,1-3H3
InchiKey: CDLRHJQHVUEVET-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CCC(C)OC(=O)CC(C)Cl
Mol. weight [g/mol]: 178.66

Physical Properties

Property code	Value	Unit	Source
gf	-234.25	kJ/mol	Joback Method
hf	-479.55	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	46.17	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.345		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1070.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1434.00		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=R28764&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