

Butanoic acid, 3-chloro, 1-methylbutyl ester

Inchi: InChI=1S/C9H17ClO2/c1-4-5-8(3)12-9(11)6-7(2)10/h7-8H,4-6H2,1-3H3
InchiKey: SEMCDZABCCWUBJ-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCC(C)OC(=O)CC(C)Cl
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-225.83	kJ/mol	Joback Method
hf	-500.19	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	48.39	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.736		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
ripol	1174.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1156.00		NIST Webbook
ripol	1162.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1511.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1519.00		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/molxK	518.16	Joback Method

cpg	366.10	J/molxK	549.24	Joback Method
cpg	378.99	J/molxK	580.32	Joback Method
cpg	391.31	J/molxK	611.40	Joback Method
cpg	403.08	J/molxK	642.48	Joback Method
cpg	414.29	J/molxK	673.56	Joback Method
cpg	424.95	J/molxK	704.64	Joback Method
dvisc	0.0058815	Paxs	263.27	Joback Method
dvisc	0.0023072	Paxs	305.75	Joback Method
dvisc	0.0011372	Paxs	348.23	Joback Method
dvisc	0.0006537	Paxs	390.72	Joback Method
dvisc	0.0004189	Paxs	433.20	Joback Method
dvisc	0.0002907	Paxs	475.68	Joback Method
dvisc	0.0002141	Paxs	518.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28746&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

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