Butanoic acid, 4-chloro, 1,1-dimethylpropyl ester

Inchi: InChI=1S/C9H17ClO2/c1-4-9(2,3)12-8(11)6-5-7-10/h4-7H2,1-3H3
InchiKey: RRLWZGBKVDJTRH-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCC(C)(C)OC(=O)CCCCl
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-218.11	kJ/mol	Joback Method
hf	-498.38	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	47.87	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.737		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1184.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1191.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1565.00		NIST Webbook
tb	515.81	K	Joback Method
tc	705.44	K	Joback Method
tf	295.69	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.29	J/mol×K	515.81	Joback Method
cpg	369.02	J/mol×K	547.41	Joback Method
cpg	382.06	J/mol×K	579.02	Joback Method
cpg	394.44	J/mol×K	610.62	Joback Method
cpg	406.18	J/mol×K	642.23	Joback Method
cpg	417.29	J/mol×K	673.83	Joback Method
cpg	427.81	J/mol×K	705.44	Joback Method
dvisc	0.0037624	Pa×s	295.69	Joback Method
dvisc	0.0018251	Pa×s	332.38	Joback Method
dvisc	0.0010222	Pa×s	369.06	Joback Method
dvisc	0.0006358	Pa×s	405.75	Joback Method
dvisc	0.0004279	Pa×s	442.44	Joback Method
dvisc	0.0003060	Pa×s	479.12	Joback Method
dvisc	0.0002295	Pa×s	515.81	Joback Method

Sources

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=R28867&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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