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

Inchi: InChI=1S/C8H15ClO2/c1-8(2,3)11-7(10)5-4-6-9/h4-6H2,1-3H3
InchiKey: CRSVVUBCNZULGK-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CC(C)(C)OC(=O)CCCCl
Mol. weight [g/mol]: 178.66

Physical Properties

Property code	Value	Unit	Source
gf	-226.53	kJ/mol	Joback Method
hf	-477.74	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	45.65	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.347		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1450.00		NIST Webbook
ripol	1458.00		NIST Webbook
tb	492.93	K	Joback Method
tc	684.84	K	Joback Method
tf	284.42	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	310.79	J/mol×K	492.93	Joback Method
cpg	323.63	J/mol×K	524.91	Joback Method
cpg	335.82	J/mol×K	556.90	Joback Method
cpg	347.40	J/mol×K	588.88	Joback Method
cpg	358.36	J/mol×K	620.87	Joback Method
cpg	368.75	J/mol×K	652.85	Joback Method
cpg	378.57	J/mol×K	684.84	Joback Method
dvisc	0.0039634	Pa×s	284.42	Joback Method
dvisc	0.0019567	Pa×s	319.17	Joback Method
dvisc	0.0011096	Pa×s	353.92	Joback Method
dvisc	0.0006964	Pa×s	388.68	Joback Method
dvisc	0.0004718	Pa×s	423.43	Joback Method
dvisc	0.0003391	Pa×s	458.18	Joback Method
dvisc	0.0002553	Pa×s	492.93	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28853&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