Butanoic acid, 3-chloro, butyl ester

Other names: Butyl 3-chlorobutanoate
n-Butyl 3-chlorobutyrate
Inchi: InChI=1S/C8H15ClO2/c1-3-4-5-11-8(10)6-7(2)9/h7H,3-6H2,1-2H3
InchiKey: CPWVMAYZTIUFPZ-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CCCCOC(=O)CC(C)Cl
Mol. weight [g/mol]: 178.66
CAS: 53815-59-1

Physical Properties

Property code	Value	Unit	Source
chl	-4695.30	kJ/mol	NIST Webbook
chl	-4704.50 ± 8.40	kJ/mol	NIST Webbook
gf	-231.81	kJ/mol	Joback Method
hf	-557.70 ± 9.60	kJ/mol	NIST Webbook
hfl	-610.90 ± 8.40	kJ/mol	NIST Webbook
hfus	19.94	kJ/mol	Joback Method
hvap	53.10 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.30		Crippen Method
logp	2.347		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1130.00		NIST Webbook
tb	495.72	K	Joback Method
tc	680.38	K	Joback Method
tf	267.00	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.89	J/mol×K	495.72	Joback Method
cpg	363.91	J/mol×K	649.60	Joback Method
cpg	353.67	J/mol×K	618.82	Joback Method
cpg	342.95	J/mol×K	588.05	Joback Method
cpg	331.75	J/mol×K	557.27	Joback Method
cpg	320.07	J/mol×K	526.50	Joback Method
cpg	373.67	J/mol×K	680.38	Joback Method
dvisc	0.0002478	Pa×s	495.72	Joback Method
dvisc	0.0003265	Pa×s	457.60	Joback Method
dvisc	0.0004523	Pa×s	419.48	Joback Method
dvisc	0.0006687	Pa×s	381.36	Joback Method
dvisc	0.0010785	Pa×s	343.24	Joback Method
dvisc	0.0019599	Pa×s	305.12	Joback Method
dvisc	0.0042242	Pa×s	267.00	Joback Method

Sources

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=C53815591&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume