Butyl 4-chlorobutanoate

Other names: Butyl 4-chlorobutanoate
n-Butyl-4-chlorobutyrate
Inchi: InChI=1S/C8H15ClO2/c1-2-3-7-11-8(10)5-4-6-9/h2-7H2,1H3
InchiKey: GKEGQZISIPAXAX-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CCCCOC(=O)CCCCl
Mol. weight [g/mol]: 178.66

Physical Properties

Property code	Value	Unit	Source
af	0.5812		Cheméo Relay (1.0)
chl	-4697.40 ± 8.40	kJ/mol	NIST Webbook
chl	-4688.60	kJ/mol	NIST Webbook
gf	-229.37	kJ/mol	Joback Method
hf	-563.60 ± 9.60	kJ/mol	NIST Webbook
hfl	-618.00 ± 8.40	kJ/mol	NIST Webbook
hfus	23.46	kJ/mol	Joback Method
hvap	54.40 ± 4.20	kJ/mol	NIST Webbook
ie	10.08	eV	Cheméo Relay (1.0)
log10ws	-2.30		Cheméo Relay (1.0)
logp	2.349		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	478.63	K	Cheméo Relay (1.0)
tc	665.85	K	Cheméo Relay (1.0)
tf	202.77	K	Cheméo Relay (1.0)
vc	0.534	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.66	J/mol×K	496.16	Joback Method
cpg	371.92	J/mol×K	677.00	Joback Method
cpg	362.34	J/mol×K	646.86	Joback Method
cpg	352.32	J/mol×K	616.72	Joback Method
cpg	341.84	J/mol×K	586.58	Joback Method
cpg	330.91	J/mol×K	556.44	Joback Method
cpg	319.52	J/mol×K	526.30	Joback Method
dvisc	0.0006370	Pa×s	389.08	Joback Method
dvisc	0.0002618	Pa×s	496.16	Joback Method
dvisc	0.0003363	Pa×s	460.47	Joback Method
dvisc	0.0004506	Pa×s	424.77	Joback Method
dvisc	0.0030458	Pa×s	282.00	Joback Method
dvisc	0.0009658	Pa×s	353.39	Joback Method
dvisc	0.0016080	Pa×s	317.69	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3153331&Units=SI

Legend

af: Acentric Factor
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
ie: Ionization energy

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