Butanoyl chloride, 4-chloro-

Other names:	«gamma»-Chlorobutyryl chloride
	4-Chlorobutyryl chloride
	4-Chlorobutyl chloride
	«gamma»-Chloro-n-butyryl chloride
	4-Chlorobutyroyl chloride
Inchi:	InChI=1S/C4H6Cl2O/c5-3-1-2-4(6)7/h1-3H2
InchiKey:	CDIIZULDSLKBKV-UHFFFAOYSA-N
Formula:	C4H6Cl2O
SMILES:	O=C(Cl)CCCCl
Mol. weight [g/mol]:	141.00
CAS:	4635-59-0

Physical Properties

Property code	Value	Unit	Source
gf	-169.98	kJ/mol	Joback Method
hf	-269.95	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	40.01	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.771		Crippen Method
mcvol	93.270	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	959.70		NIST Webbook
tb	446.70	K	NIST Webbook
tc	615.08	K	Joback Method
tf	244.61	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.74	J/mol×K	419.65	Joback Method
cpg	159.49	J/mol×K	452.22	Joback Method
cpg	165.90	J/mol×K	484.79	Joback Method

cpg	172.00	J/mol×K	517.37	Joback Method
cpg	177.79	J/mol×K	549.94	Joback Method
cpg	183.28	J/mol×K	582.51	Joback Method
cpg	188.48	J/mol×K	615.08	Joback Method
dvisc	0.0036532	Pa×s	244.61	Joback Method
dvisc	0.0020955	Pa×s	273.78	Joback Method
dvisc	0.0013378	Pa×s	302.96	Joback Method
dvisc	0.0009241	Pa×s	332.13	Joback Method
dvisc	0.0006777	Pa×s	361.30	Joback Method
dvisc	0.0005205	Pa×s	390.48	Joback Method
dvisc	0.0004147	Pa×s	419.65	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=C4635590&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume