

Butanoyl chloride, 2-chloro-

Other names:	2-Chlorobutyryl chloride
Inchi:	InChI=1S/C4H6Cl2O/c1-2-3(5)4(6)7/h3H,2H2,1H3
InchiKey:	KVQJVAOMYWTLEO-UHFFFAOYSA-N
Formula:	C4H6Cl2O
SMILES:	CCC(Cl)C(=O)Cl
Mol. weight [g/mol]:	141.00
CAS:	7623-11-2

Physical Properties

Property code	Value	Unit	Source
gf	-172.42	kJ/mol	Joback Method
hf	-275.23	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.769		Crippen Method
mcvol	93.270	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	403.70	K	NIST Webbook
tc	619.35	K	Joback Method
tf	229.61	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.85	J/mol×K	419.21	Joback Method
cpg	184.44	J/mol×K	585.99	Joback Method
cpg	178.78	J/mol×K	552.64	Joback Method
cpg	172.81	J/mol×K	519.28	Joback Method
cpg	166.50	J/mol×K	485.92	Joback Method
cpg	159.85	J/mol×K	452.57	Joback Method
cpg	189.78	J/mol×K	619.35	Joback Method
dvisc	0.0003982	Pa×s	419.21	Joback Method

dvisc	0.0005142	Pa×s	387.61	Joback Method
dvisc	0.0006946	Pa×s	356.01	Joback Method
dvisc	0.0009951	Pa×s	324.41	Joback Method
dvisc	0.0015405	Pa×s	292.81	Joback Method
dvisc	0.0026509	Pa×s	261.21	Joback Method
dvisc	0.0052966	Pa×s	229.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	324.70	K	5.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7623112&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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