

Butanoyl chloride, 4-bromo-

Other names:	4-Bromobutyryl chloride 4-Bromobutanoyl chloride «gamma»-Bromobutyryl chloride Butyryl chloride, 4-bromo- «gamma»-Bromobutyryl chloride
Inchi:	InChI=1S/C4H6BrClO/c5-3-1-2-4(6)7/h1-3H2
InchiKey:	LRTRXDSAJLSRTG-UHFFFAOYSA-N
Formula:	C4H6BrClO
SMILES:	O=C(Cl)CCCB
Mol. weight [g/mol]:	185.45
CAS:	927-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-143.73	kJ/mol	Joback Method
hf	-227.88	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	42.06	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.927		Crippen Method
mcvol	98.530	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
tb	448.38	K	Joback Method
tc	655.23	K	Joback Method
tf	274.49	K	Joback Method
vc	0.377	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.10	J/mol×K	448.38	Joback Method
cpg	166.93	J/mol×K	482.85	Joback Method
cpg	173.36	J/mol×K	517.33	Joback Method
cpg	179.43	J/mol×K	551.80	Joback Method

cpg	185.13	J/molxK	586.28	Joback Method
cpg	190.50	J/molxK	620.75	Joback Method
cpg	195.54	J/molxK	655.23	Joback Method
dvisc	0.0032909	Paxs	274.49	Joback Method
dvisc	0.0020295	Paxs	303.47	Joback Method
dvisc	0.0013616	Paxs	332.45	Joback Method
dvisc	0.0009739	Paxs	361.44	Joback Method
dvisc	0.0007321	Paxs	390.42	Joback Method
dvisc	0.0005725	Paxs	419.40	Joback Method
dvisc	0.0004622	Paxs	448.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	374.20	K	4.90	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C927582&Units=SI

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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