3-Bromopropionyl chloride

Other names:	«beta»-Bromopropionyl chloride Propanoyl chloride, 3-bromo- 3-Bromopropanoyl chloride
Inchi:	InChI=1S/C3H4BrClO/c4-2-1-3(5)6/h1-2H2
InchiKey:	IHBVNSPHKMCPST-UHFFFAOYSA-N
Formula:	C3H4BrClO
SMILES:	O=C(Cl)CCBr
Mol. weight [g/mol]:	171.42
CAS:	15486-96-1

Physical Properties

Property code	Value	Unit	Source
gf	-152.15	kJ/mol	Joback Method
hf	-207.24	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	39.84	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.537		Crippen Method
mcvol	84.440	ml/mol	McGowan Method
pc	5022.80	kPa	Joback Method
rinpol	913.00		NIST Webbook
tb	425.50	K	Joback Method
tc	634.89	K	Joback Method
tf	263.22	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.76	J/mol×K	425.50	Joback Method
cpg	130.06	J/mol×K	460.40	Joback Method
cpg	135.05	J/mol×K	495.30	Joback Method
cpg	139.73	J/mol×K	530.20	Joback Method
cpg	144.12	J/mol×K	565.09	Joback Method

cpg	148.23	J/mol×K	599.99	Joback Method
cpg	152.08	J/mol×K	634.89	Joback Method
dvisc	0.0032237	Pa×s	263.22	Joback Method
dvisc	0.0020381	Pa×s	290.27	Joback Method
dvisc	0.0013933	Pa×s	317.31	Joback Method
dvisc	0.0010111	Pa×s	344.36	Joback Method
dvisc	0.0007689	Pa×s	371.41	Joback Method
dvisc	0.0006068	Pa×s	398.45	Joback Method
dvisc	0.0004935	Pa×s	425.50	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=C15486961&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

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