

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	m ³ /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	Paxs	263.22	Joback Method
dvisc	0.0020381	Paxs	290.27	Joback Method
dvisc	0.0013933	Paxs	317.31	Joback Method
dvisc	0.0010111	Paxs	344.36	Joback Method
dvisc	0.0007689	Paxs	371.41	Joback Method
dvisc	0.0006068	Paxs	398.45	Joback Method
dvisc	0.0004935	Paxs	425.50	Joback Method

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=C15486961&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
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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