Carbonochloridic acid, 2-bromoethyl ester

Other names:	(2-Bromoethoxy)carbonyl chloride
	2-Bromoethyl chlorocarbonate
	2-Bromoethyl chloroformate
	Chloroformic acid «beta»-bromoethyl ester
	Chloroformic acid 2-bromoethyl ester
	Ethanol, 2-bromo-, chloroformate
	Formic acid, chloro-, 2-bromoethyl ester
	«beta»-Bromoethyl chloroformate
	2-Bromoethyl chloridocarbonate
Inchi:	InChI=1S/C3H4BrClO2/c4-1-2-7-3(5)6/h1-2H2
InchiKey:	ZLCKDYMZBZNBMJ-UHFFFAOYSA-N
Formula:	C3H4BrClO2
SMILES:	O=C(Cl)OCCBr
Mol. weight [g/mol]:	187.42
CAS:	4801-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-257.15	kJ/mol	Joback Method
hf	-339.46	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	42.25	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.757		Crippen Method
mcvol	90.310	ml/mol	McGowan Method
pc	4903.92	kPa	Joback Method
tb	447.92	K	Joback Method
tc	656.03	K	Joback Method
tf	285.45	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	142.74	J/mol×K	447.92	Joback Method
cpg	166.56	J/mol×K	621.34	Joback Method
cpg	162.25	J/mol×K	586.66	Joback Method
cpg	157.72	J/mol×K	551.97	Joback Method
cpg	152.96	J/mol×K	517.29	Joback Method
cpg	147.96	J/mol×K	482.60	Joback Method
cpg	170.63	J/mol×K	656.03	Joback Method
dvisc	0.0004137	Pa×s	447.92	Joback Method
dvisc	0.0005071	Pa×s	420.84	Joback Method
dvisc	0.0006392	Pa×s	393.76	Joback Method
dvisc	0.0008338	Pa×s	366.69	Joback Method
dvisc	0.0011348	Pa×s	339.61	Joback Method
dvisc	0.0016291	Pa×s	312.53	Joback Method
dvisc	0.0025049	Pa×s	285.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.70	K	1.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4801278&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