Propanoic acid, 3-bromo-2-chloro, ethyl ester

Inchi: InChI=1S/C5H8BrClO2/c1-2-9-5(8)4(7)3-6/h4H,2-3H2,1H3
InchiKey: QHNYTHIGYIAQCD-UHFFFAOYSA-N
Formula: C5H8BrClO2
SMILES: CCOC(=O)C(Cl)CBr
Mol. weight [g/mol]: 215.47

Physical Properties

Property code	Value	Unit	Source
gf	-242.75	kJ/mol	Joback Method
hf	-386.02	kJ/mol	Joback Method
hfus	17.45	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.552		Crippen Method
mcvol	118.490	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	493.24	K	Joback Method
tc	700.45	K	Joback Method
tf	292.99	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.20	J/mol×K	493.24	Joback Method
cpg	226.55	J/mol×K	527.77	Joback Method
cpg	234.49	J/mol×K	562.31	Joback Method
cpg	242.03	J/mol×K	596.84	Joback Method
cpg	249.18	J/mol×K	631.38	Joback Method
cpg	255.93	J/mol×K	665.91	Joback Method
cpg	262.31	J/mol×K	700.45	Joback Method
dvisc	0.0032213	Pa×s	292.99	Joback Method
dvisc	0.0018152	Pa×s	326.37	Joback Method
dvisc	0.0011377	Pa×s	359.74	Joback Method

dvisc	0.0007719	Pa×s	393.12	Joback Method
dvisc	0.0005566	Pa×s	426.49	Joback Method
dvisc	0.0004208	Pa×s	459.87	Joback Method
dvisc	0.0003304	Pa×s	493.24	Joback Method

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=R30296&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume