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

Inchi: InChI=1S/C7H12BrClO2/c1-5(2)4-11-7(10)6(9)3-8/h5-6H,3-4H2,1-2H3
InchiKey: REXXRTDJURMHKN-UHFFFAOYSA-N
Formula: C7H12BrClO2
SMILES: CC(C)COC(=O)C(Cl)CBr
Mol. weight [g/mol]: 243.53

Physical Properties

Property code	Value	Unit	Source
gf	-228.35	kJ/mol	Joback Method
hf	-432.58	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	50.38	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.188		Crippen Method
mcvol	146.670	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	538.56	K	Joback Method
tc	744.15	K	Joback Method
tf	300.53	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.24	J/mol×K	538.56	Joback Method
cpg	351.47	J/mol×K	709.89	Joback Method
cpg	342.70	J/mol×K	675.62	Joback Method
cpg	333.40	J/mol×K	641.36	Joback Method
cpg	323.57	J/mol×K	607.09	Joback Method
cpg	313.19	J/mol×K	572.83	Joback Method
cpg	359.73	J/mol×K	744.15	Joback Method
dvisc	0.0002522	Pa×s	538.56	Joback Method

dvisc	0.0003324	Pa×s	498.89	Joback Method
dvisc	0.0004594	Pa×s	459.22	Joback Method
dvisc	0.0006752	Pa×s	419.54	Joback Method
dvisc	0.0010753	Pa×s	379.87	Joback Method
dvisc	0.0019088	Pa×s	340.20	Joback Method
dvisc	0.0039430	Pa×s	300.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30250&Units=SI
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

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