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

Inchi: InChI=1S/C6H10BrClO2/c1-4(2)10-6(9)5(8)3-7/h4-5H,3H2,1-2H3
InchiKey: ZFRBCCORPDTTCO-UHFFFAOYSA-N
Formula: C6H10BrClO2
SMILES: CC(C)OC(=O)C(Cl)CBr
Mol. weight [g/mol]: 229.50

Physical Properties

Property code	Value	Unit	Source
gf	-236.77	kJ/mol	Joback Method
hf	-411.94	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	48.15	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.940		Crippen Method
mcvol	132.580	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
tb	515.68	K	Joback Method
tc	724.44	K	Joback Method
tf	289.26	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.37	J/mol×K	515.68	Joback Method
cpg	303.71	J/mol×K	689.65	Joback Method
cpg	295.81	J/mol×K	654.85	Joback Method
cpg	287.43	J/mol×K	620.06	Joback Method
cpg	278.58	J/mol×K	585.27	Joback Method
cpg	269.22	J/mol×K	550.47	Joback Method
cpg	311.15	J/mol×K	724.44	Joback Method
dvisc	0.0002818	Pa×s	515.68	Joback Method

dvisc	0.0003699	Pa×s	477.94	Joback Method
dvisc	0.0005086	Pa×s	440.21	Joback Method
dvisc	0.0007423	Pa×s	402.47	Joback Method
dvisc	0.0011716	Pa×s	364.73	Joback Method
dvisc	0.0020547	Pa×s	327.00	Joback Method
dvisc	0.0041723	Pa×s	289.26	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=R30317&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